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**AN INTRODUCTION TO  
THE STUDY OF WAVE MECHANICS**



# AN INTRODUCTION TO THE STUDY OF WAVE MECHANICS

BY

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# AN INTRODUCTION TO THE STUDY OF WAVE MECHANICS

## GENERAL INTRODUCTION <sup>1</sup>

THE new wave mechanics has received during the past two years the firm support of experiment, thanks to the discovery of a striking phenomenon completely unknown previously, viz.: the diffraction of electrons by crystals. From one point of view it may be said that this discovery is the exact counterpart of the older discovery of the photo-electric effect, since it shows that for matter as for light we have hitherto neglected one of the aspects of physical reality.

The discovery of the photo-electric effect has taught us that the undulatory theory of light, firmly established by Fresnel and subsequently developed by Maxwell as the electro-magnetic theory, although it contains a large body of truth, is, nevertheless, insufficient, and that it is necessary, in a certain sense, to turn again to the corpuscular conception of light proposed by Newton.

Planck, in his famous theory of black body radiation, was led to assume that radiation of frequency  $\nu$  is always emitted and absorbed in equal and finite quantities, in quanta of magnitude  $h\nu$ ,  $h$  being the constant with which the name of Planck will always be associated. In order to explain the photo-electric effect, Einstein had only to adopt the hypothesis, which is quite in conformity with the ideas of Planck, that light consists of corpuscles and that the energy of the corpuscles of light of frequency  $\nu$  is  $h\nu$ . When a light corpuscle in its passage through matter encounters an electron at rest, it can impart to it its energy  $h\nu$  and the electron thus set in

<sup>1</sup> This introduction is the reproduction of a communication made by the author at the meeting of the British Association for the Advancement of Science held in Glasgow in September, 1928.



motion will leave the matter with kinetic energy equal in amount to the difference between the energy  $h\nu$ , which it has received, and the work it has had to expend to get out of the matter. Now, this is precisely the experimental law of the photo-electric effect in the form which has been verified in succession for all the radiations from the ultra-violet region to X- and  $\gamma$ -rays.

Einstein, in developing his idea, has shown that if the hypothesis of light corpuscles or light quanta be accepted, it is necessary to attribute to each of these corpuscles a momentum  $p = \frac{h\nu}{c}$  together with energy  $W = h\nu$ . These two relations define mechanically the light corpuscle of frequency  $\nu$ . More recently the corpuscular theory of Einstein has been confirmed by the discovery of the Compton effect. This effect may be described in the following way; a beam of X-rays falling on matter may undergo a lowering of frequency, while electrons are set in more or less rapid motion. The phenomenon is readily explained if it be admitted that there is an encounter, or impact, between a light corpuscle and an electron initially at rest in the matter. During the impact the electron takes up energy from the light corpuscle and is set in motion. The light corpuscle has thus lost a part of its energy, and as the relation  $W = h\nu$  must always be maintained, the frequency of the light quantum will be less after the impact than before it. The theory of the Compton phenomenon, based on the two equations  $W = h\nu$  and  $p = \frac{h\nu}{c}$ , has been developed by Compton himself and by Debye: experiment has confirmed the theory quantitatively, and this has provided another brilliant success for the hypothesis that light has a granular structure.

In spite of these successes the theory of light quanta would not by itself be completely satisfactory. In the first place, those phenomena described by the terms diffraction and interference demand the introduction of the concept of waves, and, further, the two relations  $W = h\nu$  and  $p = \frac{h\nu}{c}$  imply the existence of a frequency  $\nu$ .

This is sufficient to show that light cannot consist of simple

But if for a century we have neglected too much the corpuscular aspect in the theory of light in our exclusive attachment to waves, have we not erred in the opposite direction in the theory of matter? Have we not wrongly neglected the point of view of waves and thought only of corpuscles? These are the questions the author of this book set himself some years ago in reflecting upon the analogy between the principle of least action and the principle of Fermat and upon the meaning of the mysterious quantum conditions introduced into intra-atomic dynamics by Planck, Bohr, Wilson and Sommerfeld.

$$W = \frac{mc^2}{\sqrt{1-\beta^2}}, \quad p = \frac{mv}{\sqrt{1-\beta^2}} = \frac{Wv}{c^2}, \quad \left(\beta = \frac{v}{c}\right), \quad (1)$$

According to the new conception it is necessary to associate with this particle a wave travelling in the direction of motion of which the frequency is:

$$\nu = \frac{W}{h} \quad (2)$$

$$V = \frac{c^2}{v} = \frac{c}{\beta}, \quad (3)$$
$$\frac{h\nu}{V} = \frac{W}{c^2}v = p \quad (4)$$

If we seek to apply these formulæ, not only to a material particle but also to a light particle, we must write  $v = c$ , and then we find :

These are exactly the fundamental formulæ of the theory of light quanta. Our formulæ (2) to (5) are thus general; they apply equally well to matter and radiation, and they are the expression of the necessity in both cases of introducing side by side the ideas of corpuscle and of wave.

As follows, in particular, from the elegant works of Schrödinger, and as we shall show in detail in the course of these studies, the old mechanics corresponds to the case in which the propagation of the associated wave proceeds according to the laws of geometrical optics. In this case the corpuscle or particle may be regarded as describing one of the rays of the wave with a velocity equal to Lord Rayleigh's group velocity. Thus we may under these circumstances consider the particle as constituted by a group of waves of neighbouring frequencies and this gives a physical picture of the particle which would be very satisfactory were it possible to generalise it; unfortunately, this is not the case.

It is to be noted that, if the associated wave is propagated according to the laws of geometrical optics no experiment can prove the existence of associated waves, because the result of an experiment can then always be regarded as proving only the exactness of the laws of the old mechanics. But it is quite another matter when the conditions of propagation of the associated wave are such that the approximations of geometrical optics are no longer sufficiently accurate to describe the process. According to the new ideas, we must then expect to observe phenomena which the old mechanics is quite powerless to predict and which are characteristic of the new undulatory conception of dynamics.

In the domain proper to the new dynamics, the principle

which appears best established is that the square of the amplitude of the wave, i.e. its intensity, must measure at each point of space and at each instant of time the probability that the associated particle is at that point at that instant. A little reflection will show that this principle is necessary to account for the phenomena of interference and diffraction of light, for in optics the maximum luminous energy is found in the places where the Fresnel wave has the greatest intensity. Since we are following as our guide the idea of bringing together as closely as possible the theory of light and that of matter, it is quite natural to extend the principle which is necessary in the case of light to the case of particles of matter.

We thus arrive at the idea that material particles will give rise to phenomena analogous to those of interference and diffraction of light and that the methods of calculation must be closely alike in the two cases. Thus a cloud consisting of electrons with the same velocity must be associated with a plane monochromatic wave. Let us suppose that this cloud falls on a medium with regular structure, such as occurs in the case of a crystal. If the distances between the elements of this structure are of the same order of magnitude as the wavelength of the incident wave, diffraction will occur, and in certain directions, which may be readily found by calculation, the amplitude of the diffracted wave will have maximum values. In accordance with this, we must expect that the electrons will be concentrated along certain directions. We shall thus have the exact analogy with Laue's experiment on X-rays, and if the result agrees with the theoretical deduction we shall obtain a very direct and a very strong proof that it is necessary, even in the case of matter, to complete our conception of a particle by the addition of that of a wave.

These experiments have been realised by various methods under different conditions by Davisson and Germer in New York, by Professor G. P. Thompson in Aberdeen, and by Rupp in Göttingen. The agreement between theory and experiment is excellent; the deviations which had been established in the first experiments of Davisson and Germer appear to receive a very natural explanation by taking account of the refractive index of the waves in the crystal. Rupp has, indeed, been able quite recently to diffract a beam of electrons at grazing

incidence on an ordinary lined grating. Thus, experimental confirmation is as satisfactory as could be desired.

In this way a collection of magnificent experimental results has clearly established the necessity of introducing simultaneously particles and waves into the whole domain of physics.

But what does this duality of waves and particles mean? This is a very difficult question and one which is still far from being very clearly elucidated.

The simplest idea is that which Schrödinger put forward at the beginning of his work, viz. that the particle or the electron is constituted by a group of waves; it is a "wave packet." We have seen that this can be maintained so long as mechanical phenomena are considered which are in harmony with the old dynamics, that is to say in the new language, phenomena in which the propagation of the associated wave obeys the laws of geometrical optics. Unfortunately, when we pass to the domain proper of the new theory it appears scarcely possible to support this idea which is so attractive on account of its simplicity. In an experiment like that of the diffraction of an electron by a crystal the wave packet would be completely dispersed and destroyed; as a result no particles would be found in the diffracted bundles. In other words, if they were simple wave packets the particles would have no stable existence.

If it appears impossible to maintain Schrödinger's view in all its consequences, neither is it easy to develop another opinion with which the author has for a long time associated himself and according to which the particle is a singularity in a wave phenomenon. In the special case of the uniform motion of a particle it is possible to find a solution of the wave equation showing a moving singularity and capable of representing the particle. But it is very difficult to make the generalisation to the case of non-uniform motion, and there are serious objections to this point of view; we shall not discuss this difficulty any further in this volume.

The author has also made another suggestion which is published in his report to the Fifth Solway Congress.<sup>1</sup> We have seen that we must always associate a wave with a

<sup>1</sup> "Electrons et photons," Gauthier Villars, editeur, Paris, 1928.

particle, and so the idea which is in best agreement with the older views of physics is to consider the wave as a reality and as occupying a certain region of space, while the particle is regarded as a material point having a definite position in the wave. This is the basis of the suggestion. Since it is necessary, as we have said above, that the intensity of the wave should be proportional at each point to the probability of the occurrence of the particle at that point, we must attempt to connect the motion of the particle with the propagation of the wave so that this relation is automatically realised in every case. It is, in fact, actually possible to establish a connection between the motion of the particle and the propagation of the wave, so that if at an initial instant the intensity of the wave measures the required probability the same is true at all later instants. We may thus suppose that the particle is guided by the wave which plays the part of a pilot-wave. This view permits of an interesting visualization of the corpuscular motion in wave mechanics without too wide a departure from classical ideas. Unfortunately, we encounter very serious objections to this view also, and these will be pointed out in the course of the book. It is not possible to regard the theory of the pilot-wave as satisfactory. Nevertheless, since the equations on which this theory rests are sound, we may preserve some of its consequences by giving to it a modified form in agreement with ideas developed independently by Kennard.<sup>1</sup> Instead of speaking of the motion and of the trajectory of the particles, we speak of the motion and of the trajectory of the "elements of probability" and in this way the difficulties noted are avoided.

Finally, there is a fourth point of view developed by Heisenberg and Bohr which is most favoured at present. This point of view is a little disconcerting at first sight, but yet it appears to contain a large body of truth. According to this view, the wave does not represent a physical phenomenon taking place in a region of space; rather it is simply a symbolic representation of what we know about the particle. An experiment or observation never permits us to say exactly that this particle occupies this position in space and that it has this particular velocity. All that experiment can show us

<sup>1</sup> "Physical Review," 31, 1928, p. 876.

is that the position and velocity of the particle lie within certain limits, or, in other words, that there is a certain probability that the particle lies in a particular position and some other probability that it has a particular velocity. The information that an initial experiment or observation made at time  $t_0$  gives may be represented symbolically by a wave of which the intensity at  $t_0$  gives the probability of occurrence of the particle at any point and of which the spectral distribution gives the relative probability of the various states of motion. If we study the propagation of the wave from the instant  $t_0$  to a later instant  $t$ , the partition of intensity and the spectral distribution at the instant  $t$  will allow us to say what the probability is that a second experiment or observation, made at the instant  $t$ , will localise the particle at a particular point or ascribe to it a particular state of motion.

The essential consequence of this point of view is Heisenberg's uncertainty relation. A limited wave train can only be considered appreciably monochromatic if its dimensions are large with respect to the wave-length. If, therefore, as the result of an observation, we localise the particle in a region of space which is of small dimensions with respect to the wave-length, it will have to be represented by a wave train which is by no means monochromatic. Thus, from Heisenberg's point of view, the more precisely we attempt to determine the position the less accurately can we determine the state of motion. Conversely, the more exactly the state of motion is defined the more closely will the associated wave approach a plane monochromatic wave with constant amplitude. Thus the more exactly the state of motion is defined the less definite will be the estimation of the position of the particle. Bohr states that there are two complementary aspects of reality; localisation in space-time and dynamical specification by energy and momentum. It is as if there were two different planes and it were impossible to focus exactly on both at the same time. For illustration let it be supposed that there is a diagram of which certain parts are drawn in a plane  $\Pi$  and other parts in a plane  $\Pi'$  very close to  $\Pi$  and parallel to it. If we examine this diagram with a not too precise optical instrument we shall succeed, by focussing on a plane between  $\Pi$  and  $\Pi'$ , in obtaining an image in fair agreement with the diagram,

and we shall have the impression that it is all traced in one plane. But if we use an optical instrument of great accuracy, the more carefully we focus on  $\Pi$  the more blurred will be the parts traced on  $\Pi'$  and we shall recognise that the diagram is not all traced on one plane.

The old mechanics is the analogy of the inaccurate optical instrument; under its guidance we had the illusion that we could determine at one and the same time both the position and state of motion of the particle. But with the new mechanics, which is the analogy of the accurate instrument, we are compelled to recognize that localisation in space and time and energy specification are two different planes of reality which it is impossible to bring clearly into focus simultaneously. This, it appears, is the fundamental conception of Bohr and Heisenberg.

This leads to the consequence already foreseen by Born that we can no longer assert that there is a rigorous determinism in Nature, for all the determinism of the old dynamics rested on the possibility of determining simultaneously the initial position and velocity of a particle, which is impossible if Heisenberg's view is admitted. Consequently there are no longer any rigorous laws, but only laws of probability.

This method of interpreting wave mechanics introduces many surprises. In the first place, the particles have existence, and we admit that in speaking of their number we are giving expression to something which has a definite meaning. But with Bohr's ideas it is no longer possible to hold the clear and classic picture which portrays them as very small objects having position in space, a velocity and a trajectory. In the second place, the other party in this dualism, the wave, is no more than a purely symbolic and analytic representation of certain probabilities, and no longer constitutes a physical phenomenon in the old meaning of the term. An example will make this last point clear. Let us suppose that at the time  $t$  the wave train associated with a particle occupies a region  $R$  of space, and that a particular observation made at this instant permits us to state that the particle is to be found in a region  $R'$  which is naturally within  $R$ ; then the wave packet must be "reduced," to use Heisenberg's expression, that is to say, the whole of the wave within  $R$  but external to



$R'$  vanishes just as the expectation of an event which is not realized vanishes. This shows very clearly the non-physical character of the wave in the conceptions of Bohr and Heisenberg.

To sum up, the physical interpretation of the new mechanics remains an extremely difficult question. Nevertheless, one great fact is now well established ; this is that for matter and for radiation the dualism of waves and particles must be admitted, and that the distribution of the particles in space can only be foreseen by the consideration of waves. Unfortunately the profound nature of the two members in this duality and the precise relation existing between them still remain a mystery.

## CHAPTER I

### THE OLD SYSTEMS OF MECHANICS OF A PARTICLE

#### 1. Hamilton's Principle

THERE are two systems of mechanics which we may describe under the term "old mechanics." The first of these, and the older of the two, is the classical or Newtonian mechanics; the second is the relativistic mechanics of Einstein. Newtonian mechanics remained for a long time sufficient for the needs of science, but the profound conceptions of Einstein have shown that it must be modified so that a system is obtained which coincides with the older when the velocity of the particle is small compared with the velocity,  $c$ , of light in empty space, but which deviates from it when the velocity is comparable with  $c$ .

The two old systems of mechanics, in spite of the differences between them, at the same time resemble one another in important particulars; the general equations have the same form, they are both derivable from the same principle, that of least action, and there are other analogies. For this reason it is easy to describe at the same time the general principles of the two systems. The essential point is that all the formulæ of Newtonian mechanics can be deduced from the mechanics of Einstein by supposing that the velocity of light in empty space is infinitely great; in other words, the classical formulæ are always obtained from the relativity formulæ by a development in a series in powers of  $\beta (= \frac{v}{c})$  and by omitting the terms of higher orders.

We shall consider first the dynamics of a single particle, that is to say, we shall study the motion of a particle in a field of force which is assumed to be given. We shall define this

field of force by a potential function  $F(x, y, z, t)$  of the co-ordinates of space and time. In the old mechanics we consider particles or corpuscles as having a definite position in space so that we can record their position by means of three co-ordinates. Thus, since the particle has a definite situation in space at each instant, we may evidently define its velocity as the limit of the ratio of the space described along the trajectory and the time taken when the latter tends to zero. If the position of the particle is recorded by means of rectangular co-ordinates, we have :

$$v = \sqrt{\dot{x}^2 + \dot{y}^2 + \dot{z}^2},$$

where the dots denote differentiation with respect to time. In the general case, where curvilinear co-ordinates ( $q_1, q_2, q_3$ ) are employed, the velocity is expressed by a certain function of the  $q$ 's and  $\dot{q}$ 's.

The fundamental principle of the two old dynamics is Hamilton's principle of stationary action. Let it be supposed that at the instant  $t_0$  the particle is situated at a point  $M_0$  of space and that at a later instant  $t_1$  it is at  $M_1$ . The problem arising in the dynamics of a particle is to determine the motion in the interval of time between  $t_0$  and  $t_1$ . Hamilton's principle states that a certain function  $L(q, \dot{q}, t)$  exists, which is a function of the  $q$ 's,  $\dot{q}$ 's, and the time, with the property that the integral  $\int_{t_0}^{t_1} L dt$  is smaller for the actual motion than for any other infinitesimally varied motion which takes the particle from  $M_0$  at time  $t_0$  to  $M_1$  at time  $t_1$ .

The integral  $\int_{t_0}^{t_1} L dt$  is the Hamiltonian integral of action. The function  $L$  is called the Lagrangian function and sometimes the kinetic potential.

Hamilton's principle of least action is thus described by the formula :

$$\delta \int_{t_0}^{t_1} L(q, \dot{q}, t) dt = 0, \quad . \quad . \quad . \quad (1)$$

$t_0$  and  $t_1$  being invariable, and the symbol denoting an infinitesimal change in the form of the function  $q(t)$ , and consequently in  $\dot{q}(t)$ , with the condition that their initial and final values are unchanged.

## 2. The Equations of Lagrange

The general procedure of the calculus of variations will lead to the equations of Lagrange. If we change the function  $q$  for each value of  $t$  so that it becomes  $q + \delta q$ , the function  $\dot{q}$  will become  $\dot{q} + \delta \dot{q}$ , and we obtain :

$$\delta L = \sum_{n=1}^{n=3} \left( \frac{\partial L}{\partial q_n} \delta q_n + \frac{\partial L}{\partial \dot{q}_n} \delta \dot{q}_n \right) \quad . \quad . \quad (2)$$

and in consequence, since  $t_0$  and  $t_1$  are fixed,

$$\delta \int_{t_0}^{t_1} L dt = \int_{t_0}^{t_1} \delta L dt = \int_{t_0}^{t_1} \sum_{n=1}^{n=3} \left( \frac{\partial L}{\partial q_n} \delta q_n + \frac{\partial L}{\partial \dot{q}_n} \delta \dot{q}_n \right) dt = 0. \quad (3)$$

But  $\delta \dot{q} = \delta \left( \frac{dq}{dt} \right) = \frac{d}{dt} (\delta q)$ , so that by integration by parts,

$$\int_{t_0}^{t_1} \sum_{n=1}^{n=3} \frac{\partial L}{\partial \dot{q}_n} \delta \dot{q}_n dt = \left[ \sum_{n=1}^{n=3} \frac{\partial L}{\partial \dot{q}_n} \delta q_n \right]_{t_0}^{t_1} - \int_{t_0}^{t_1} \sum_{n=1}^{n=3} \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_n} \right) \delta q_n dt, \quad (4)$$

whence we obtain for Hamilton's principle (1) :

$$\int_{t_0}^{t_1} \sum_{n=1}^{n=3} \delta q_n \left[ \frac{\partial L}{\partial q_n} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_n} \right) \right] dt = 0. \quad . \quad . \quad (5)$$

Since the  $\delta q$ 's are arbitrary, it follows that :

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_n} \right) - \frac{\partial L}{\partial q_n} = 0 \quad (n = 1, 2, 3). \quad . \quad . \quad (6)$$

These are the equations of Lagrange. They define the motion of the particle as a function of 6 arbitrary constants which may be the three initial co-ordinates and the three components of the initial velocity.

## 3. The Lagrangian Function. Momentum and Energy

Up to this point our dynamical theory has remained, as it were, a blank form, since we have not stated the form of the function  $L$  in the  $q$ 's,  $\dot{q}$ 's and  $t$ . It is just at this point that the mechanics of Newton and Einstein diverge in that the choice of  $L$  is different.

In the Newtonian system

$$L(q, \dot{q}, t) = \frac{1}{2}mv^2 - F(q, t), \quad . \quad . \quad (7)$$

$m$  being a characteristic constant of the particle considered, called its mass. The function  $F(q, t)$  is the potential function, and  $v$  is the velocity of the particle which must be expressed in terms of the  $q$ 's and  $\dot{q}$ 's.

In Einstein's system

$$L(q, \dot{q}, t) = -mc^2\sqrt{1 - \beta^2} - F(q, t). \quad . \quad (8)$$

Since  $\sqrt{1 - \beta^2} = 1 - \frac{1}{2}\beta^2 + \dots$ , we see that by neglecting the unwritten terms, we have :

$$L = -mc^2 + \frac{1}{2}mv^2 - F(q, t), \quad . \quad . \quad (9)$$

so that the relativistic form of the function with this degree of approximation differs from the classical form only in the constant term  $-mc^2$ . In the integral (1) this term gives rise to  $-mc^2(t_1 - t_0)$ , which is not subject to variation and may consequently be neglected. In this way we readily appreciate the point mentioned above that these two systems of mechanics coincide when we neglect the higher powers of  $\beta$ .

Now that we know how we must fill in our blank Hamiltonian form in order to obtain the one or the other old system of dynamics, let us return to the equations of Lagrange.

We shall define certain quantities  $p$  by the equations :

$$p_n = \frac{\partial L}{\partial \dot{q}_n} \quad (n = 1, 2, 3) \quad . \quad . \quad (10)$$

and we shall describe  $p_n$  as the conjugate momentum of  $q_n$ .

The equations of Lagrange then give :

$$\frac{dp_n}{dt} = \frac{\partial L}{\partial q_n}. \quad . \quad . \quad . \quad (11)$$

Let us consider briefly the particular case where the co-ordinates are rectangular. We have then :

$$q_1 = x, \quad q_2 = y, \quad q_3 = z, \quad \text{and} \quad v^2 = \dot{x}^2 + \dot{y}^2 + \dot{z}^2.$$

With the Newtonian form of  $L$  we find :

$$p_1 = m\dot{x}, \quad p_2 = m\dot{y}, \quad p_3 = m\dot{z}. \quad . \quad . \quad (12)$$

The  $p$ 's are thus the components of the momentum  $m\mathbf{v}$ . With the relativistic form of  $L$ ,

$$p_1 = \frac{m\dot{x}}{\sqrt{1-\beta^2}}, \quad p_2 = \frac{m\dot{y}}{\sqrt{1-\beta^2}}, \quad p_3 = \frac{m\dot{z}}{\sqrt{1-\beta^2}}. \quad (13)$$

The  $p$ 's will then be components of momentum if this quantity is defined to be equal to

$$\frac{m\mathbf{v}}{\sqrt{1-\beta^2}}.$$

Moreover, in both cases the choice of rectangular co-ordinates has the effect of making  $L$  depend upon the  $q$ 's only through the function  $F$ . Hence :

$$\frac{\partial L}{\partial q} = -\frac{\partial F}{\partial q}. \quad . \quad . \quad . \quad (14)$$

If we consider the vector  $-\text{grad } F$  with components

$$\left(-\frac{\partial F}{\partial x}, \quad -\frac{\partial F}{\partial y}, \quad -\frac{\partial F}{\partial z}\right),$$

and if we call this vector the force applied to the particle, denoting it by  $\mathbf{f}$ , the equations (11) give the classical equations :

$$\frac{dp_1}{dt} = f_x, \quad \frac{dp_2}{dt} = f_y, \quad \frac{dp_3}{dt} = f_z \quad . \quad . \quad (15)$$

which are applicable in both the old dynamical systems.

Let us now introduce the conception of energy. For this purpose we begin with the general formal expression of the equations of Lagrange :

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_n}\right) = \frac{dp_n}{dt} = \frac{\partial L}{\partial q_n}. \quad (n = 1, 2, 3) \quad . \quad (16)$$

Now let us consider the quantity :

$$W = \sum_{n=1}^{n=3} p_n \dot{q}_n - L, \quad . \quad . \quad . \quad (17)$$

and obtain its time derivative :

$$\frac{dW}{dt} = \sum_{n=1}^{n=3} \left[ \dot{q}_n \frac{dp_n}{dt} + p_n \frac{d\dot{q}_n}{dt} - \frac{\partial L}{\partial q_n} \dot{q}_n - \frac{\partial L}{\partial \dot{q}_n} \cdot \frac{d\dot{q}_n}{dt} \right] - \frac{\partial L}{\partial t}. \quad (18)$$

The first and third terms of the right-hand side of (18) cancel on account of the equations of Lagrange, the second and fourth on account of the definition of  $p_n$ . Thus :

$$\frac{dW}{dt} = - \frac{\partial L}{\partial t}, \quad . \quad . \quad . \quad (19)$$

whence the theorem ; if the function  $L$  does not depend explicitly on the time, the quantity  $W$  remains constant.  $W$  is called the energy of the particle.

Let us examine the expression for the energy in classical dynamics. We have in this case  $L = \frac{1}{2}mv^2 - F$ , and whatever the co-ordinates chosen, the term  $\frac{1}{2}mv^2$  is a homogeneous quadratic function of the  $\dot{q}$ 's for  $v^2 = \dot{x}^2 + \dot{y}^2 + \dot{z}^2$ , and each of the terms  $\dot{x}$ ,  $\dot{y}$ ,  $\dot{z}$  is a linear function of the  $\dot{q}$ 's. Thus, if  $T = \frac{1}{2}mv^2$ , we obtain, by means of Euler's theorem,

$$2T = \sum_{n=1}^{n=3} \dot{q}_n \frac{\partial T}{\partial \dot{q}_n} = \sum_{n=1}^{n=3} \dot{q}_n \frac{\partial L}{\partial \dot{q}_n} = \sum_{n=1}^{n=3} p_n \dot{q}_n, \quad . \quad (20)$$

since  $L$  depends on the  $\dot{q}$ 's through  $T$  only.

We therefore obtain :

$$W = 2T - L = 2T - (T - F) = T + F. \quad . \quad (21)$$

The energy is the sum of  $T(= \frac{1}{2}mv^2)$ , called the kinetic energy, and of  $F$ , called the potential energy.

Let us pass now to the dynamics of relativity where

$$L = - mc^2 \sqrt{1 - \beta^2} - F.$$

We can no longer follow exactly the same argument, since  $\sqrt{1 - \beta^2}$  is not a homogeneous quadratic function of the  $\dot{q}$ 's, but we can write :

$$\sum_{n=1}^{n=3} p_n \dot{q}_n = \sum_{n=1}^{n=3} \dot{q}_n \frac{\partial L}{\partial \dot{q}_n} = \sum_{n=1}^{n=3} \dot{q}_n \frac{m}{2\sqrt{1 - \beta^2}} \frac{\partial v^2}{\partial \dot{q}_n} \quad . \quad (22)$$

and since  $v^2$  is a homogeneous quadratic function of the  $\dot{q}_n$ 's, we have :

$$2v^2 = \sum_{n=1}^{n=3} \dot{q}_n \frac{\partial v^2}{\partial \dot{q}_n}$$

and by (22) :

$$\sum_{n=1}^{n=3} p_n \dot{q}_n = \frac{mv^2}{\sqrt{1-\beta^2}} \quad . \quad . \quad . \quad (23)$$

Thus :

$$\begin{aligned} W = \sum_{n=1}^{n=3} p_n \dot{q}_n - L &= \frac{mv^2}{\sqrt{1-\beta^2}} + mc^2 \sqrt{1-\beta^2} + F \\ &= \frac{mc^2}{\sqrt{1-\beta^2}} + F. \quad (24) \end{aligned}$$

The term  $\frac{mc^2}{\sqrt{1-\beta^2}}$  represents the energy of the particle in motion in the dynamics of relativity. If the particle is at rest the term has the value  $mc^2$ , which is the energy of the particle at rest, that is, its internal energy corresponding to its rest mass  $m$  and equal to the product of the rest mass and the square of the velocity of light. When the particle is in motion this energy becomes  $\frac{mc^2}{\sqrt{1-\beta^2}}$ , which is equal to the product of  $c^2$  and the quantity  $\frac{m}{\sqrt{1-\beta^2}}$ , which may be regarded as the mass of the particle in motion. It is important to note that a particle with a proper mass different from zero must always have a speed lower than that of light, since its energy tends to infinity when  $\beta$  tends to unity.

If we develop  $\frac{mc^2}{\sqrt{1-\beta^2}}$  in a series of powers of  $\beta$ , neglecting higher powers, we find :

$$W = mc^2 + \frac{1}{2}mv^2 + F \quad . \quad . \quad . \quad (25)$$

and we see that the relativistic energy is to this degree of approximation equal to that of Newtonian mechanics increased by the term  $mc^2$ . We must never lose sight of this essential difference, and must remember that classical dynamics systematically neglects the internal energy term  $mc^2$ .

#### 4. Another form of Hamilton's Principle. The Principle of Maupertuis

We proceed to show that it is possible to give to Hamilton's integral of action the form of an integral along a curve. For



this purpose let us consider an abstract four dimensional space formed by the union of the three co-ordinates  $q$  and the time  $t$ . The motion of the particle is represented in this space by a certain curve, since this motion is expressed by three relations of the type :

$$q_n = f_n(t).$$

This curve is what is called in the theory of relativity the world line of the moving particle ; along this curve each co-ordinate  $q_n$  is a certain function of the time.

By (17) Hamilton's integral may be written :

$$\int_{P_0}^{P_1} \left( \sum_{n=1}^{n=3} p_n dq_n - W dt \right), \quad . \quad . \quad . \quad (26)$$

the points  $P_0$  and  $P_1$  corresponding to the times  $t_0$  and  $t_1$  on the world line. The principle of stationary action asserts that this line integral is stationary for all infinitely small deformations from the curve of integration, the extremities of the curve being kept fixed, which means that neither the initial and final instants nor the initial and final positions are varied.

In the case of constant fields of force the principle of stationary action takes a particularly important form. In fact, we have :  $\frac{\partial F}{\partial t} = 0$ , and consequently  $\frac{\partial L}{\partial t} = 0$ . The energy is constant, and we can give to the principle a celebrated form of expression which is due to Maupertuis. This permits of the determination of the trajectory without the necessity of considering the way in which the particle describes it. It is only for fields of force which are constant in time that such a separation between the study of the trajectory and the study of the motion can be realised ; this may be readily understood by the following consideration.

To pass from Hamilton's principle, which is always true, to the principle of Maupertuis, which is restricted to constant fields, it is necessary to establish a formula sometimes called the principle of varied action. Instead of considering a variation in which the initial and final times and co-ordinates are fixed, let us cause them to vary also by very small amounts  $\delta t_0$ ,  $\delta t_1$  and  $(\delta q_n)_0$ ,  $(\delta q_n)_1$ . The variation of Hamilton's integral

is the sum of what it would be if the limits were not varied and of the variation due to change of the limits.

Thus :

$$\delta \int_{t_0}^{t_1} L dt = \int_{t_0}^{t_1} \delta L dt + \left[ \sum_{n=1}^{n=3} p_n \delta q_n - W \delta t \right]_0^1 \quad . \quad (27)$$

for when the initial instant is varied by  $\delta t_0$  and the initial co-ordinates by  $(\delta q_n)_0$ , the integral, considered as a line integral, evidently changes by

$$- \left[ \sum_{n=1}^{n=3} (p_n)_0 (\delta q_n)_0 - W_0 \delta t_0 \right],$$

while for variations at the upper limit, the change is

$$+ \left[ \sum_{n=1}^{n=3} (p_n)_1 (\delta q_n)_1 - W_1 \delta t_1 \right].$$

The first term of (27) is zero according to Hamilton's principle, so that :

$$\delta \int_{t_0}^{t_1} L dt = \left[ \sum_{n=1}^{n=3} p_n \delta q_n - W \delta t \right]_0^1 \quad . \quad . \quad (28)$$

This formula is the expression of the principle of varied action. Denote by  $S$  Hamilton's integral, and by  $S_1$  the curvilinear integral,

$$\text{i.e.} \quad S_1 = \int_{M_0}^{M_1} \sum_{n=1}^{n=3} p_n dq_n \quad . \quad . \quad . \quad (29)$$

taken along the trajectory from the initial point  $M_0$  to the final point  $M_1$ . The integral (29) is the integral of action of Maupertuis. Since in the case of a constant field the formulæ (21) and (24) allow the velocity, and consequently the  $p$ 's, to be expressed as a function of the constant energy and of the co-ordinates  $q$ , the integral of Maupertuis does not depend upon the time. We have :

$$S = S_1 - \int_{t_0}^{t_1} W dt \quad . \quad . \quad . \quad (30)$$

and consequently in general for any variation whatsoever :

$$\delta S = \delta S_1 - \int_{t_0}^{t_1} \delta W dt - \left[ W \delta t \right]_0^1. \quad (31)$$

By comparison with (28) we find :

$$\delta S_1 = \left[ \sum_{n=1}^{n=3} p_n \delta q_n \right]_0^1 + \int_{t_0}^{t_1} \delta W dt. \quad (32)$$

If, therefore, we restrict ourselves to variations of the trajectory in which the ends  $M_0$  and  $M_1$  are unchanged, while the energy is unaltered, the integral of action of Maupertuis is stationary. This is the principle of Maupertuis.

Let us consider the case where the  $q$ 's are rectangular co-ordinates so that :

$$\sum_{n=1}^{n=3} p_n dq_n = p_x dx + p_y dy + p_z dz \quad (33)$$

and we see that the integral  $S_1$  has the following interpretation. It is the integral of momentum along the trajectory, and has the value  $\int m v ds$  in classical mechanics and  $\int \frac{mv}{\sqrt{1-\beta^2}} ds$  in relativistic mechanics,  $ds$  denoting the element of arc of the trajectory.

## 5. The Hamiltonian Canonical Equations

We proceed to show that the dynamical equations can be put into a form well known as Hamilton's canonical equations. Since the function  $L$  depends on the  $q$ 's,  $\dot{q}$ 's and  $t$ , we may, by means of (10), express the  $p$ 's as a function of these variables, and consequently write in general :

$$\dot{q}_n = f_n(q, p, t), \quad (n = 1, 2, 3) \quad (34)$$

where  $f_n$  denotes a function which can be calculated in any particular case.

We may thus choose as our variables the  $q$ 's,  $p$ 's and  $t$  in the place of the  $q$ 's,  $\dot{q}$ 's and  $t$ . Let  $H(q, p, t)$  denote the energy expressed in terms of these variables which are often described

as the canonical variables. We have by the definition of energy :

$$H(q, p, t) = \sum_{n=1}^{n=3} p_n \dot{q}_n - L(q, \dot{q}, t), \quad . \quad . \quad (35)$$

where, on the right-hand side, we must suppose that the  $\dot{q}$ 's are expressed as functions of the  $p$ 's,  $q$ 's and  $t$  by means of (34). If we determine the derivatives  $\frac{\partial H}{\partial p_m}$  and  $\frac{\partial H}{\partial q_m}$ , where  $m$  has a definite value 1, 2 or 3,

$$\begin{aligned} \frac{\partial H}{\partial p_m} &= \dot{q}_m + \sum_{n=1}^{n=3} p_n \frac{\partial f_n}{\partial p_m} - \sum_{n=1}^{n=3} \frac{\partial L}{\partial \dot{q}_n} \frac{\partial f_n}{\partial p_m} \\ &= \dot{q}_m \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (36) \end{aligned}$$

$$\begin{aligned} \frac{\partial H}{\partial q_m} &= \sum_{n=1}^{n=3} p_n \frac{\partial f_n}{\partial q_m} - \frac{\partial L}{\partial q_m} - \sum_{n=1}^{n=3} \frac{\partial L}{\partial \dot{q}_n} \frac{\partial f_n}{\partial q_m} \\ &= -\frac{\partial L}{\partial q_m} = -\frac{dp_m}{dt} \text{ by the equations of Lagrange. } (37) \end{aligned}$$

We have thus obtained the system of Hamiltonian canonical equations :

$$\frac{dq_n}{dt} = \frac{\partial H}{\partial p_n}, \quad \frac{dp_n}{dt} = -\frac{\partial H}{\partial q_n} \quad (n = 1, 2, 3) \quad . \quad (38)$$

It is easy to deduce the theorem of conservation of energy, and it suffices to determine  $\frac{dH}{dt}$ .

$$\begin{aligned} \frac{dH}{dt} &= \frac{\partial H}{\partial t} + \sum_{n=1}^{n=3} \left( \frac{\partial H}{\partial p_n} \frac{dp_n}{dt} + \frac{\partial H}{\partial q_n} \frac{dq_n}{dt} \right) \\ &= \frac{\partial H}{\partial t} \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (39) \end{aligned}$$

According to the definition of energy given in (35), it appears that if  $L$  does not contain the time explicitly, the same is true of  $H$  and  $\frac{\partial H}{\partial t} = 0$ . Thus the energy is constant, a result already obtained.

We proceed to consider in detail Hamilton's equations in both the old systems of dynamics.

Let us take first the case of classical mechanics with rectangular co-ordinates.

We have :

$$p_x = mv_x, \quad p_y = mv_y, \quad p_z = mv_z, \\ v^2 = v_x^2 + v_y^2 + v_z^2 = \frac{1}{m^2}(p_x^2 + p_y^2 + p_z^2), \quad . \quad . \quad (40)$$

whence

$$H = \frac{1}{2}mv^2 + F = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + F(q, t). \quad (41)$$

The equations  $\frac{dq_n}{dt} = \frac{\partial H}{\partial p_n}$  are immediately verified, since we have, for example :

$$\frac{dx}{dt} = v_x = \frac{p_x}{m} = \frac{\partial H}{\partial p_x}. \quad . \quad . \quad (42)$$

The equations  $\frac{dp_n}{dt} = -\frac{\partial H}{\partial q_n}$  now become :

$$m\frac{dv_x}{dt} = -\frac{\partial F}{\partial x}, \text{ etc.} \quad . \quad . \quad (43)$$

These are the fundamental Newtonian equations.

Let us now take the relativity theory with rectangular axes.

In this case :

$$p_x = \frac{m}{\sqrt{1-\beta^2}}v_x, \quad p_y = \frac{m}{\sqrt{1-\beta^2}}v_y, \quad p_z = \frac{m}{\sqrt{1-\beta^2}}v_z, \quad (44)$$

$$H = \frac{mc^2}{\sqrt{1-\beta^2}} + F(q, t). \quad . \quad . \quad (45)$$

It is necessary first of all to express  $H$  as a function of the  $q$ 's,  $p$ 's and  $t$ .

We have :

$$p_x^2 + p_y^2 + p_z^2 = \frac{m^2v^2}{1-\beta^2},$$

whence

$$\frac{1}{m^2c^2}(p_x^2 + p_y^2 + p_z^2) = \frac{\beta^2}{1-\beta^2}. \quad . \quad . \quad (46)$$

If we add unity to each side and take the square root, we obtain :

$$\frac{1}{\sqrt{1-\beta^2}} = \frac{1}{mc} \sqrt{m^2c^2 + p_x^2 + p_y^2 + p_z^2} \quad . \quad (47)$$

and

$$H(q, p, t) = c \sqrt{m^2c^2 + p_x^2 + p_y^2 + p_z^2} + F(q, t) \quad (48)$$

We have therefore :

$$\frac{\partial H}{\partial q_n} = \frac{\partial F}{\partial q_n}, \quad \frac{\partial H}{\partial p_n} = \frac{cp_n}{\sqrt{m^2c^2 + \sum_1^3 p_n^2}} = \frac{p_n}{m} \sqrt{1-\beta^2}, \quad (49)$$

where the suffixes 1, 2, 3 are to be identified with  $x, y, z$  respectively. The equations  $\frac{dq_n}{dt} = \frac{\partial H}{\partial p_n}$  are again identically satisfied in this case, since we have :

$$\frac{dx}{dt} = v_x = \frac{p_x}{m} \sqrt{1-\beta^2}, \text{ etc.} \quad . \quad . \quad (50)$$

The equations  $\frac{dp_n}{dt} = -\frac{\partial H}{\partial q_n}$  give the equations of motion of the dynamics of Einstein's theory :

$$\frac{d}{dt} \left[ \frac{mv_x}{\sqrt{1-\beta^2}} \right] = -\frac{\partial F}{\partial x}, \text{ etc.} \quad . \quad . \quad (51)$$

## 6. Contact Transformations

Hamilton's equations are expressed in terms of seven variables, the time  $t$ , the three co-ordinates  $q_n$ , and the three momenta  $p_n$ . Let the variables  $q_n$  and  $p_n$  be replaced by new variables  $\alpha_n$  and  $\beta_n$  ( $n = 1, 2, 3$ ), defined by relations such as :

$$\alpha_n = f_n(p, q, t), \quad \beta_n = \phi_n(p, q, t). \quad . \quad . \quad (52)$$

We do not at present attribute any particular dynamical significance to the  $\alpha$ 's and  $\beta$ 's, they are merely six new variables. The relations (52) may be written :

$$p_n = F_n(\alpha, q, t), \quad \beta_n = \Phi_n(\alpha, q, t). \quad . \quad . \quad (53)$$

We may then obtain the theorem that if it is possible to find a function  $S(\alpha, q, t)$  such that :

$$\sum_{n=1}^{n=3} p_n dq_n - \sum_{n=1}^{n=3} \beta_n d\alpha_n = - (dS)_t, \quad . \quad . \quad (54)$$

where  $(dS)_t$  denotes a variation in which  $t$  is constant, then the variables  $\alpha$  and  $\beta$  satisfy the canonical equations :

$$\frac{d\alpha_n}{dt} = \frac{\partial K}{\partial \beta_n}, \quad \frac{d\beta_n}{dt} = - \frac{\partial K}{\partial \alpha_n} \quad (n = 1, 2, 3) \quad . \quad (55)$$

where  $K = H - \frac{\partial S}{\partial t}$ .

In order to prove this, we note that

$$\frac{\partial S}{\partial \alpha_n} = \beta_n, \quad \frac{\partial S}{\partial q_n} = - p_n, \quad (dS)_t = dS - \frac{\partial S}{\partial t} dt \quad . \quad (56)$$

and in consequence, by (54),

$$\begin{aligned} \sum_{n=1}^{n=3} p_n dq_n - H dt &= \sum_{n=1}^{n=3} \beta_n d\alpha_n - H dt - dS + \frac{\partial S}{\partial t} dt \quad (57) \\ &= \sum_{n=1}^{n=3} \beta_n d\alpha_n - K dt - dS. \end{aligned}$$

Let the initial and final positions be characterised by times  $t_0$  and  $t_1$  and by co-ordinates  $(q_n)_0$  and  $(q_n)_1$  respectively.

Consider space of four dimensions in which the co-ordinates are the four variables  $(q_n, t)$ . Hamilton's principle shows that if the motion of the particle is represented in this space by a curve  $C$  joining  $M_0$  with co-ordinates  $(q_n)_0, t$  and  $M_1$  with co-ordinates  $(q_n)_1, t$ , the integral

$$\int_{M_0}^{M_1} \left( \sum_{n=1}^{n=3} p_n dq_n - H dt \right)$$

taken along this curve does not vary to the first order of small quantities if the curve is deformed while keeping  $M_0$  and  $M_1$  fixed. We have :

$$\int_{M_0}^{M_1} \delta \left( \sum_{n=1}^{n=3} p_n dq_n - H dt \right) = 0.$$

Let us consider also the four-dimensional space formed by the time and the three variables  $x_n$ . A curve  $\Gamma$  in this new space then corresponds to the curve  $C$ , for at each point of the latter there are definite values, not only of  $q_n$  and  $t$ , but also of  $p_n$ ; in consequence, by (52), each point of  $C$  corresponds to a point of  $\Gamma$ . Let  $(\alpha_n)_0$  at  $t_0$ , and  $(\alpha_n)_1$  at  $t_1$  be the co-ordinates of the extremities of  $\Gamma$ . When the curve  $C$  is varied with fixed extremities in order to apply Hamilton's principle, the curve  $\Gamma$  varies in consequence, but in general its extremities are not fixed, since the initial and final values of the  $p$ 's are, in general, affected by the variation of  $C$ , and on this account a change occurs in  $(\alpha_n)_0$  and  $(\alpha_n)_1$ .

Thus :

$$\int_{(q_n)_0}^{(q_n)_1} \delta \left( \sum_{n=1}^{n=3} p_n dq_n - H dt \right) = \int_{(\alpha_n)_0}^{(\alpha_n)_1} \delta \left( \sum_{n=1}^{n=3} \beta_n d\alpha_n - K dt \right) + \left[ \sum_{n=1}^{n=3} \beta_n d\alpha_n \right]_0^1 - \delta [S]_0^1 \quad (58)$$

since  $\int_0^1 dS = [S]_0^1$ , and since the  $q_0$ 's and the  $q_1$ 's are fixed, we have :

$$\delta [S]_0^1 = \left[ \sum_{n=1}^{n=3} \frac{\partial S}{\partial \alpha_n} \delta \alpha_n \right]_0^1 . \quad . \quad . \quad (59)$$

The last two terms of (58) cancel one another by (56) and (59), and finally :

$$\int_{(q_n)_0}^{(q_n)_1} \delta \left( \sum_{n=1}^{n=3} p_n dq_n - H dt \right) = \int_{(\alpha_n)_0}^{(\alpha_n)_1} \delta \left( \sum_{n=1}^{n=3} \beta_n d\alpha_n - K dt \right), \quad (60)$$

where the variation of the right-hand side is subject to the condition that the initial and final values of the  $\alpha$ 's are fixed. Since the left-hand side is zero by Hamilton's principle, the same is true of the right-hand side, and since the  $\beta$ 's,  $\alpha$ 's, and the function  $K$  play the same part as the  $p$ 's,  $q$ 's and  $H$ , we conclude that the equations (55) are verified.

In short we may say that the change of variables expressed by (54), and known as a contact transformation, preserves the form of Hamilton's equations, provided that the original  $H$  is replaced by  $K = H - \frac{\partial S}{\partial t}$ .



## CHAPTER II

### THE THEORY OF JACOBI

#### 1. The Equation of Jacobi

**T**HE theorem on contact transformations will enable us to obtain at once the Jacobian equation. Let it be supposed that we have found a contact transformation such that  $K = 0$ . Then the new canonical variables  $\alpha_n$  and  $\beta_n$  will satisfy the Hamiltonian equations :

$$\frac{d\alpha_n}{dt} = 0, \quad \frac{d\beta_n}{dt} = 0. \quad (n = 1, 2, 3) \quad . \quad . \quad . \quad (1)$$

The  $\alpha$ 's and  $\beta$ 's will thus be constants. Now  $K$  is equal to  $H - \frac{\partial S}{\partial t}$ , and  $p_n$  to  $-\frac{\partial S}{\partial q_n}$ . Thus, by expressing the energy in terms of the  $q$ 's,  $p$ 's and  $t$ , and by replacing  $p_n$  by  $-\frac{\partial S}{\partial q_n}$ , the condition  $K = 0$  is equivalent to :

$$H(q, -\frac{\partial S}{\partial q}, t) = \frac{\partial S}{\partial t}. \quad . \quad . \quad . \quad (2)$$

This first order equation in the partial derivatives of  $S$  is the equation of Jacobi. If an integral of this equation is found containing three arbitrary constants,  $\alpha_n$ , that is to say, the complete integral of (2), this function  $S(q_n, \alpha_n, t)$  will define a contact transformation between the variables  $q_n, p_n, t$  and the quantities  $\alpha_n, \beta_n \left( = \frac{\partial S}{\partial \alpha_n} \right), t$  with  $K = 0$ .

We have :

$$\alpha_n = \text{constant}, \quad \beta_n = \frac{\partial S}{\partial \alpha_n} = \text{constant}. \quad . \quad (3)$$

We may thus derive Jacobi's theorem that if it is possible to find a complete integral  $S(q, \alpha, t)$  of the first order partial differential equation :

$$H(q, -\frac{\partial S}{\partial q}, t) = \frac{\partial S}{\partial t} \quad . \quad . \quad . \quad (4)$$

we shall have :

$$p_n = \frac{\partial S}{\partial q_n}, \quad \frac{\partial S}{\partial \alpha_n} = \beta_n. \quad . \quad . \quad . \quad (5)$$

The  $\beta$ 's being three new constants, the equations (5), which define the six quantities  $q_n, p_n$  as functions of the time and the six constants  $\alpha_n, \beta_n$ , give completely the motion of the particle.

## 2. Hamilton's Integral and Jacobi's Function

In the theory of contact transformations given above, the variables  $\alpha_n, \beta_n$  are six variables, of which the dynamical significance is not defined. We can thus suppose that the  $\alpha$ 's are co-ordinates, the  $\beta$ 's being the momenta. Since the  $\alpha$ 's are constants in the function  $S(q, \alpha, t)$ , we are naturally led to consider them as initial co-ordinates of the particle. In order to examine this in detail let us consider not a single particle but a cloud of identical particles, all situated in the same field of force and without mutual reactions. The motion of this cloud, taken altogether, represents a whole assembly of possible motions of the same particle in the given field. The motion of the cloud between the instant  $t_0$  and the instant  $t$  has the effect of transforming the initial co-ordinates  $(q_n)_0$  of the particles of the cloud at time  $t_0$  to the final co-ordinates  $(q_n)$  at the instant  $t$ .

Let us now consider Hamilton's integral :

$$I = \int \left( \sum_{n=1}^{n=3} p_n dq_n - H dt \right)$$

along the trajectory of the particle from  $(q_n)_0$  to  $q_n$ . It is a function of the co-ordinates  $q_n, (q_n)_0$ , and of the time which satisfies the equations :

$$\frac{\partial I}{\partial q_n} = p_n, \quad \frac{\partial I}{\partial (q_n)_0} = - (p_n)_0, \quad . \quad . \quad . \quad (6)$$

the quantities  $(p_n)_0$  denoting the initial values of the  $p$ 's. The function  $I$  with its sign changed thus defines a contact transformation between the variables  $q_n$ ,  $p_n$ , and the variables  $(q_n)_0$ ,  $(p_n)_0$ . Moreover, the function  $S(q, (q)_0, t) = -I$  satisfies Jacobi's equation, for

$$S(q, (q)_0, t) = \int_0^1 \left( H dt - \sum_{n=1}^{n=3} p_n dq_n \right) \quad . \quad (7)$$

and consequently :

$$\frac{\partial S}{\partial t} = H(q, p, t), \quad \frac{\partial S}{\partial q_n} = -p_n, \quad . \quad . \quad (8)$$

thus :

$$\frac{\partial S}{\partial t} = H\left(q, -\frac{\partial S}{\partial q}, t\right) \quad . \quad . \quad . \quad (9)$$

According to Jacobi's theorem the co-ordinates  $(q_n)_0$  must be constants in the course of the motion, which is in agreement with their character as initial values of the co-ordinates, and the quantities  $(p_n)_0$  must therefore be constants; they are the initial momenta.

### 3. The Reduced Function of Jacobi

The  $\alpha$ 's are not necessarily the values of the initial co-ordinates. We can also find a complete integral depending upon the initial momenta, or even of other constants.

Whenever such an integral is found, we have :

$$p_n = -\frac{\partial S}{\partial q_n}, \quad \frac{\partial S}{\partial \alpha_n} = \beta_n = \text{constant} \quad . \quad . \quad (10)$$

and these equations will determine the motion.

A special case of importance is that of constant fields. In this case, as we have seen, the energy is constant. Denoting this constant by  $W$ , the Hamiltonian integral is

$$\int \left( \sum_{n=1}^{n=3} p_n dq_n - W dt \right),$$

and if we adopt for  $S$  this integral with the sign changed we have :

$$\frac{\partial S}{\partial t} = W.$$

Moreover, if we write :

$$S_1 = \int \sum_{n=1}^{n=3} p_n dq_n \quad . \quad . \quad . \quad (11)$$

we have :

$$S = Wt - S_1, \quad \frac{\partial S}{\partial q_n} = - \frac{\partial S_1}{\partial q_n} \quad . \quad . \quad (12)$$

Finally,  $H$  does not contain the time explicitly, so that  $S_1$ , which we call the reduced function of Jacobi, satisfies the equation :

$$H\left(q, \frac{\partial S_1}{\partial q}\right) = W. \quad . \quad . \quad . \quad (13)$$

If a complete integral, which will depend upon  $W$  and two arbitrary constants  $\alpha_1$  and  $\alpha_2$ , be found for (13), the function  $S = Wt - S_1(q, \alpha_1, \alpha_2, W)$  will be a complete integral with three arbitrary constants  $\alpha_1, \alpha_2, \alpha_3 (= W)$  of the complete Jacobian equation, and from Jacobi's theorem we know that the motion is defined by the relations :

$$p_n = \frac{\partial S_1}{\partial q_n}, \quad \frac{\partial S_1}{\partial \alpha_1} = -\beta_1 = \text{constant}, \quad \frac{\partial S_1}{\partial \alpha_2} = -\beta_2 = \text{constant},$$

$$\frac{\partial S}{\partial W} = t - \frac{\partial S_1}{\partial W} = -\beta_3 = \text{constant}. \quad (14)$$

Let us write  $\beta_3 = -t_0$ , so that the last equation gives

$$\frac{\partial S_1}{\partial W} = t - t_0. \quad . \quad . \quad . \quad (15)$$

This equation, the only one that contains the time, gives the law of motion, while the two equations:  $\frac{\partial S_1}{\partial \alpha_1} = \text{const.}$  and  $\frac{\partial S_1}{\partial \alpha_2} = \text{const.}$  depend upon the  $q$ 's, and define the form of the trajectory. Here we find the separation of the study of the motion and the study of the trajectory which is characteristic of constant fields.

#### 4. Different Forms of Jacobi's Equation

Before studying concrete examples, we will consider in detail the form that Jacobi's equation takes in classical

mechanics and in the mechanics of Einstein, taking the classical case first. For the sake of generality we suppose the co-ordinates chosen are of any kind whatsoever. In classical mechanics the kinetic energy  $T$  is a homogeneous quadratic function of the velocities  $\dot{q}$ .

Thus :

$$T = \frac{1}{2} \sum m_{kl} \dot{q}_k \dot{q}_l, \quad . \quad . \quad . \quad (16)$$

where the summation is actually double and extends over the values (1, 2, 3) for  $k$  and  $l$ , and where  $m_{kl} = m_{lk}$ , these being functions of the  $q$ 's only. From (16) we deduce :

$$L = T - F = \frac{1}{2} \sum m_{kl} \dot{q}_k \dot{q}_l - F(q, t) \quad . \quad . \quad (17)$$

$$W = T + F = \frac{1}{2} \sum m_{kl} \dot{q}_k \dot{q}_l + F(q, t) \quad . \quad . \quad (18)$$

By definition :

$$p_n = \frac{\partial L}{\partial \dot{q}_n} = \sum_{k=1}^{k=3} m_{kn} \dot{q}_k. \quad (n = 1, 2, 3) \quad . \quad (19)$$

If we solve the linear equations (19) with respect to the  $\dot{q}$ 's, we find :

$$\dot{q}_n = \sum_{k=1}^{k=3} \frac{M_{kn}}{|m_{kl}|} p_k \quad (n = 1, 2, 3) \quad . \quad . \quad (20)$$

where  $|m_{kl}|$  denotes the determinant formed by the coefficients  $m_{kl}$ , and where  $M_{kn}$  denotes the minor corresponding to the element  $m_{kn}$  of this determinant.

$$\text{Let us write} \quad \frac{M_{kn}}{|m_{kl}|} = m^{kn},$$

so that :

$$\dot{q}_n = \sum_{k=1}^{k=3} m^{kn} p_k. \quad (n = 1, 2, 3) \quad . \quad . \quad (21)$$

Replacing the  $\dot{q}$ 's by the values (21), and substituting in (16) we find :

$$T = \frac{1}{2} \sum m_{kl} m^{kn} p_n m^{lr} p_r, \quad . \quad . \quad . \quad (22)$$

where the summation is to be made over the values (1, 2, 3) for  $k, l, n$  and  $r$ . By the properties of determinants :

$$\sum_{k=1}^{k=3} m_{kl} m^{kn} = \sum_{k=1}^{k=3} m_{kl} \frac{M_{kn}}{|m_{kl}|} = 1 \text{ or } 0, \quad . \quad . \quad (23)$$

according as  $l = n$  or  $l \neq n$ .

Thus :

$$T = \frac{1}{2} \sum m^{lr} p_l p_r, \quad . \quad . \quad . \quad (24)$$

where, again, the summation is a double one over  $l$  and  $r$ .

Consequently the energy expressed as a function of the  $q$ 's,  $p$ 's and  $t$  is :

$$H(q, p, t) = \frac{1}{2} \sum m^{lr} p_l p_r + F(q, t). \quad . \quad . \quad (25)$$

We then obtain for Jacobi's equation :

$$\frac{\partial S}{\partial t} = \frac{1}{2} \sum m^{lr} \frac{\partial S}{\partial q_l} \frac{\partial S}{\partial q_r} + F(q, t). \quad . \quad . \quad (26)$$

In the special case of rectangular co-ordinates we have :

$$T = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \quad . \quad . \quad . \quad (27)$$

so that :

$$m_{kk} = m, \quad m_{kl} = 0, \quad \text{when } k \neq l.$$

Hence :

$$m^{kk} = \frac{1}{m}, \quad m^{kl} = 0, \quad \text{for } k \neq l, \quad . \quad . \quad (28)$$

and Jacobi's equation takes the simple classical form :

$$\frac{\partial S}{\partial t} = \frac{1}{2m} \left[ \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + \left( \frac{\partial S}{\partial z} \right)^2 \right] + F(x, y, z, t) \quad (29)$$

Let us now pass to the dynamics of relativity. As we shall not make many applications of these dynamics in this work we will limit ourselves to the case of rectangular co-ordinates. We have found (Chap. I (48)) :

$$H(q, p, t) = c \sqrt{m^2 c^2 + p_x^2 + p_y^2 + p_z^2} + F(x, y, z, t). \quad (30)$$

This expression for  $H$  leads to the relativity equation of Jacobi :

$$\frac{\partial S}{\partial t} = c \sqrt{m^2 c^2 + \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + \left( \frac{\partial S}{\partial z} \right)^2} + F(x, y, z, t), \quad (31)$$

$$\frac{1}{c^2} \left( \frac{\partial S}{\partial t} - F \right)^2 - \left( \frac{\partial S}{\partial x} \right)^2 - \left( \frac{\partial S}{\partial y} \right)^2 - \left( \frac{\partial S}{\partial z} \right)^2 = m^2 c^2. \quad (32)$$

### 5. Jacobi's Function in the case of Uniform Rectilinear Motion

We proceed to find the form of Jacobi's function in two simple and important cases, which will be useful later on. We will content ourselves with classical dynamics and begin with the case of the uniform rectilinear motion of a particle in the absence of a field. Thus  $F = 0$  and equation (29) becomes :

$$\frac{1}{2m} \left[ \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + \left( \frac{\partial S}{\partial z} \right)^2 \right] = \frac{\partial S}{\partial t}. \quad (33)$$

It is easy to verify that a complete integral is given by :

$$S(x, y, z, x_0, y_0, z_0, t) = -\frac{m}{2t} [(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2]. \quad (34)$$

By Jacobi's theorem we have :

$$p_x = -\frac{\partial S}{\partial x} = \frac{m}{t}(x - x_0) \quad (35)$$

and

$$\frac{\partial S}{\partial x_0} = \frac{m}{t}(x - x_0) = \text{constant}, \quad (36)$$

with similar equations in  $y$  and  $z$ .

The constants occurring are thus equal to the constant values of  $p_x$ ,  $p_y$ ,  $p_z$  and the equations of the motion take the well-known form :

$$x = x_0 + v_x t, \quad y = y_0 + v_y t, \quad z = z_0 + v_z t. \quad (37)$$

It appears that the three arbitrary constants  $x_0$ ,  $y_0$ ,  $z_0$  of the complete integral are in this case the three co-ordinates of the particle at  $t = 0$ . The integral (34) is simply Hamilton's integral with the sign changed. We can, in fact, write Hamilton's integral in the form :

$$\int_0^t T dt = \int_0^t \frac{1}{2} m v^2 dt = \frac{1}{2} m v^2 t \quad (38)$$

Now, since the motion is uniform,

$$v_x = \frac{x - x_0}{t}, \quad v_y = \frac{y - y_0}{t}, \quad v_z = \frac{z - z_0}{t} \quad (39)$$

and

$$v^2 = v_x^2 + v_y^2 + v_z^2 = \frac{1}{t^2}[(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2]. \quad (40)$$

It thus appears that Hamilton's integral is exactly (34) with the opposite sign.

In the case of no field we can also find a complete integral of Jacobi's equation where the arbitrary constants are the three momenta, which are in this case constant, instead of the three initial co-ordinates. This complete integral is :

$$S(x, y, z, t, p_x, p_y, p_z) = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)t - p_x x - p_y y - p_z z. \quad (41)$$

The equations  $\frac{\partial S}{\partial x} = p_x$ , etc., are identically satisfied. The other three Jacobian relations are :

$$\frac{\partial S}{\partial p_x} = \frac{1}{m}p_x t - x = \text{constant}, \quad . \quad . \quad (42)$$

together with the equations in  $y$  and  $z$ .

If we denote the three constants by  $-x_0$ ,  $-y_0$ ,  $-z_0$ , we obtain again the equations of motion (37). The solution (41) may be derived also from Hamilton's integral, since for the latter, except for an additive constant, we have in this case :

$$p_x x + p_y y + p_z z - Wt.$$

Since

$$p_x = mv_x, \quad p_y = mv_y, \quad p_z = mv_z,$$

and

$$W = \frac{1}{2}mv^2 = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2),$$

Hamilton's integral with change of sign gives (41).

Finally, we have seen that in constant fields, where the field alone plays a dominant part, we could write Jacobi's function in the form  $Wt - S_1(x, y, z, \alpha_1, \alpha_2, W)$ ,  $S_1$  being an integral of equation (13). In order to put the function in this form we shall note that it is possible to express one of the momenta, for example  $p_z$ , in terms of  $W$  and the other two, since

$$p_z^2 = 2mW - p_x^2 - p_y^2. \quad . \quad . \quad (43)$$



By substituting this value of  $p_z$  into Hamilton's integral with the sign changed, we obtain :

$$S(x, y, z, t, W, p_x, p_y) = Wt - p_x x - p_y y - z\sqrt{2mW - p_x^2 - p_y^2} \quad (44)$$

and

$$S_1(x, y, z, p_x, p_y, W) = p_x x + p_y y + z\sqrt{2mW - p_x^2 - p_y^2}. \quad (45)$$

The equations of motion (14) and (15) give :

$$\left. \begin{aligned} \frac{\partial S_1}{\partial p_x} &= x - \frac{p_x z}{\sqrt{2mW - p_x^2 - p_y^2}} = \text{constant, with a similar} \\ &\text{equation in } y, \\ \text{and} \\ \frac{\partial S_1}{\partial W} &= \frac{mz}{\sqrt{2mW - p_x^2 - p_y^2}} = t - t_0 \end{aligned} \right\} \quad (46)$$

The first two give the rectilinear trajectories defined by

$$\frac{x - x_0}{p_x} = \frac{y - y_0}{p_y} = \frac{z - z_0}{p_z}. \quad (47)$$

The third equation of (46) defines the motion on the trajectory, i.e. it gives  $z$  as a function of  $t$  :

$$z = \frac{t - t_0}{m} \sqrt{2mW - p_x^2 - p_y^2} = \frac{p_z}{m}(t - t_0), \quad (48)$$

where  $t_0$  evidently denotes the time corresponding to  $y = 0$ .

## 6. Jacobi's Function in a Uniform Constant Field

Let us now take the case which, after that of no field, is next in order of simplicity. This is the case where a uniform constant field exists. Let  $k_x$ ,  $k_y$ ,  $k_z$ , denote the force components, which have the same values everywhere.

Then

$$F(x, y, z) = - \sum k_x x, \quad (49)$$

since  $f_x = - \frac{\partial F}{\partial x} = k_x$ , and there are similar equations in  $y$  and  $z$ .

Jacobi's equation in this case is :

$$\frac{1}{2m} \left[ \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + \left( \frac{\partial S}{\partial z} \right)^2 \right] - \sum k_x x = \frac{\partial S}{\partial t} . \quad (50)$$

The following is a complete integral of this equation :

$$S(x, y, z, t, x_0, y_0, z_0) = -\frac{m}{2t} \sum (x - x_0)^2 - \frac{1}{2} t \sum k_x (x + x_0) + \frac{1}{24m} t^3 \sum k_x^2 . \quad (51)$$

It is easy to verify this solution by substitution, and we find, from the equations of Jacobi's theory,

$$p_x = -\frac{\partial S}{\partial x} = \frac{m}{t}(x - x_0) + \frac{1}{2} k_x t . \quad (52)$$

together with similar equations in  $y$  and  $z$ .

These equations may be verified, since in the case of uniformly-accelerated motion we have :

$$x = x_0 + v_{0x}t + \frac{1}{2} \frac{k_x}{m} t^2 . \quad (53)$$

and

$$v_x = v_{0x} + \frac{k_x}{m} t, \quad (54)$$

again with similar equations in  $y$  and  $z$ .

From these :

$$p_x = mv_x = \frac{m}{t}(x - x_0) + \frac{1}{2} k_x t,$$

which is the same as (52).

The other three relations :  $\frac{\partial S}{\partial \alpha_n} = \text{constant}$ , are in this particular case :

$$\frac{\partial S}{\partial x_0} = \frac{m}{t}(x - x_0) - \frac{1}{2} k_x t = \text{constant} . \quad (55)$$

and the similar equations in  $y$  and  $z$ .

If  $x_0, y_0, z_0$  are initial co-ordinates,  $\frac{\partial S}{\partial x_0}, \frac{\partial S}{\partial y_0}, \frac{\partial S}{\partial z_0}$  the initial momenta  $mv_{0x}, mv_{0y}, mv_{0z}$ , and we obtain equations (53) for uniformly-accelerated motion,  $\{ -p_z^2 \}^{\frac{1}{2}}$ . (68)

We will now show that the complete integral (51) can be obtained from Hamilton's integral. The latter, with a change of sign, is in fact :

$$\int (Wdt - \sum p_x dx) = \int \left[ \left( \frac{1}{2}mv^2 - \sum k_x x \right) dt - \sum mv_x dx \right] \quad (56)$$

where the integration extends from the initial to the final time and position.

But the formulæ (53) and (54) for uniformly accelerated motion give :

$$v^2 = v_x^2 + v_y^2 + v_z^2 = \sum \left( \frac{x - x_0}{t} + \frac{1}{2} \frac{k_x t}{m} \right)^2 \quad (57)$$

and substituting in (56) we find, for the right-hand side :

$$\int \left[ \left\{ \frac{1}{2}m \sum \left( \frac{x - x_0}{t} + \frac{1}{2} \frac{k_x t}{m} \right)^2 - \sum k_x x \right\} dt - \sum m \left( \frac{x - x_0}{t} + \frac{1}{2} \frac{k_x t}{m} \right) dx \right]. \quad (58)$$

We note that the coefficient of  $dt$  when partially differentiated with respect to  $x$  gives the result obtained by differentiating the coefficient of  $dx$  partially with respect to  $t$ , and a similar remark is true for those of  $dy$  and  $dz$ . Thus the quantity under the sign of integration is a perfect differential. On evaluating the integral, we find that it has the value (51) so that, except for the sign, (51) is equal in this case also to Hamilton's integral.

As in the case of uniform motion, we can obtain a complete integral of Jacobi's equation, in which the three arbitrary constants are the initial momenta instead of the initial co-ordinates. These initial momenta are :

$$p_{0x} = mv_{0x}, \quad p_{0y} = mv_{0y}, \quad p_{0z} = mv_{0z}. \quad (59)$$

If we again change the sign of Hamilton's integral and make use of the equations (54), we obtain :

Then  $\int \left[ \left\{ \frac{1}{2m} \sum (p_{0x} + k_x t)^2 - \sum k_x x \right\} dt - \sum (p_{0x} + k_x t) dx \right]. \quad (60)$

condition of integrability is verified at once, since :

since  $f_x = - \left\{ \frac{1}{2m} \sum (p_{0x} + k_x t)^2 - \sum k_x x \right\} = -k_x = - \frac{\partial}{\partial t} (p_{0x} + k_x t) \quad (61)$

with similar equations in  $y$  and  $z$ , and the integral (60) has the value :

$$S(x, y, z, t, p_{0x}, p_{0y}, p_{0z}) = \frac{1}{6m} \sum \frac{(p_{0x} + k_x t)^3}{k_x} - \sum (p_{0x} + k_x t)x \quad (62)$$

We may easily verify a result which follows from the second paragraph of this chapter, i.e. that the function (62) satisfies Jacobi's equation (50). The equations  $p_n = \frac{\partial S}{\partial q_n}$  are identically satisfied, because of the manner in which (62) was obtained. The equations  $\frac{\partial S}{\partial \alpha_n} = \text{constant}$  give :

$$\frac{\partial S}{\partial p_{0x}} = \frac{1}{2m} \frac{(p_{0x} + k_x t)^2}{k_x} - x, \quad . \quad . \quad (63)$$

with the equations in  $y$  and  $z$ .

Since  $\frac{p_{0x}^2}{2mk_x}$ ,  $\frac{p_{0y}^2}{2mk_y}$ ,  $\frac{p_{0z}^2}{2mk_z}$  are constants, we can also write :

$$x = \frac{p_{0x}}{m}t + \frac{1}{2} \frac{k_x}{m} t^2 + \text{constant}, \quad . \quad . \quad (64)$$

and similar expressions for  $y$  and  $z$ , and obtain again the classical equations (53). Finally, we seek a complete integral of (50) having the form :

$$S(x, y, z, t, \alpha_1, \alpha_2, W) = Wt - S_1(x, y, z, \alpha_1, \alpha_2, W), \quad (65)$$

which we know is possible, since the field is constant in time. We shall obtain this function by once more calculating Hamilton's integral and changing the sign, but to simplify the calculations we will take the direction of the uniform field as the axis of  $x$ . Then  $k_y = k_z = 0$ , and the momenta  $p_y$  and  $p_z$  are constant. The energy expression

$$W = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) - k_x x, \quad . \quad . \quad (66)$$

gives us :

$$p_x = \sqrt{2m(W + k_x x) - p_y^2 - p_z^2}, \quad . \quad . \quad (67)$$

and consequently the negative Hamilton integral is :

$$\begin{aligned} Wt - \int (p_x dx + p_y dy + p_z dz) \\ = Wt - p_y y - p_z z - \int \sqrt{2m(W + k_x x) - p_y^2 - p_z^2} dx \\ = Wt - p_y y - p_z z - \frac{1}{3mk_x} \{2m(W + k_x x) - p_y^2 - p_z^2\}^{\frac{3}{2}}. \end{aligned} \quad (68)$$

By equating this to (65) we deduce :

$$S_1(x, y, z, \alpha_1, \alpha_2, W) = p_y y + p_z z \\ + \frac{1}{3mk_x} \{2m(W + k_x x) - p_y^2 - p_z^2\}^{\frac{3}{2}}, \quad (69)$$

where

$$p_y = \alpha_1, \quad p_z = \alpha_2.$$

The other expressions of the theory give :

$$\frac{\partial S_1}{\partial p_y} = y - \frac{p_y}{mk_x} \sqrt{2m(W + k_x x) - p_y^2 - p_z^2} = \text{constant}, \quad (70)$$

and a similar expression for  $\frac{\partial S_1}{\partial p_z}$ . These define the trajectory, which in this case is a parabola.

Also

$$\frac{\partial S_1}{\partial W} = \frac{1}{k_x} \sqrt{2m(W + k_x x) - p_y^2 - p_z^2} = t - t_0, \quad (71)$$

or

$$p_x = k_x(t - t_0) \equiv k_x t + p_{0x}, \quad (72)$$

where  $p_{0x}$  denotes the initial value of  $p_x$ , and the equation gives the well-known relation between the velocity and time (cf. 54).

## CHAPTER III

### THE CONCEPTIONS UNDERLYING WAVE MECHANICS

#### 1. The Point of Departure

THE point of departure in wave mechanics was the wish always to associate the idea of a particle with that of periodicity in such a way as to bind inseparably the idea of the motion of a particle with that of wave propagation.

We shall first examine the simplest case, that of a corpuscle moving freely outside any field of force, and we shall see that the connection to be established between wave and particle is then in some measure imposed by the fundamental principles of relativity.

We remind ourselves in the first place that a Galilean system of axes is a rectangular system at rest or in uniform rectilinear motion with respect to the fixed stars ; it is for systems of this kind that the equations of dynamics are valid. The principle of inertia, which is of the nature of a definition in disguise, teaches that if a particle is subject to no forces it is necessarily at rest or in uniform rectilinear motion in a Galilean system.

Of the infinite number of Galilean systems let us consider two in particular. The first with respect to which the particle possesses the velocity  $v$  ( $= \beta c$ ) is so oriented that the particle describes the axis of  $z$ . The second, called the "proper system" of the particle, moves with respect to the first with the velocity  $\mathbf{v}$  in magnitude and direction, and its  $z$  axis slides over that of the first system. We will denote by  $x_0, y_0, z_0$  the co-ordinates of a point in the proper system, while  $x, y, z$  denote those of the point in the second system.

Before Einstein's theory came into being the existence of an absolute time was accepted with the property that an observer bound to the system  $(x, y, z)$  was supposed to make

use of the same time co-ordinate as an observer bound to the proper system. The variables of space and time were therefore supposed to be related by the Galilean group of formulæ :

$$x = x_0, \quad y = y_0, \quad z = z_0 + vt, \quad t = t_0. \quad (1)$$

The profound researches of Einstein have led us to think that it is necessary to substitute instead of (1) the following Lorentz group :

$$x = x_0, \quad y = y_0, \quad z = \frac{z_0 + vt_0}{\sqrt{1 - \beta^2}}, \quad t = \frac{t_0 + \frac{\beta}{c}z_0}{\sqrt{1 - \beta^2}}, \quad (2)$$

from which we deduce inversely :

$$x_0 = x, \quad y_0 = y, \quad z_0 = \frac{z - vt}{\sqrt{1 - \beta^2}}, \quad t_0 = \frac{t - \frac{\beta}{c}z}{\sqrt{1 - \beta^2}}. \quad (3)$$

We shall adopt the formulæ (2) and (3) without entering here into any further discussion of the ideas of the theory of relativity, which would be out of place in the present work.

Let us place ourselves in the system of reference  $(x_0, y_0, z_0)$  which is bound to the particle. Since it is our aim to associate a wave with the particle, it is quite natural to suppose that this wave has the form of a stationary wave in the proper system, that is to say, that its mathematical expression depends only on the time through a factor  $\cos 2\pi\nu_0(t_0 - \tau_0)$ , and we can place  $\tau_0 = 0$ , since this depends only upon a convenient choice of the origin in time. We shall describe the constant  $\nu_0$  by the term "proper frequency" of the particle.

Let us now change our point of view by placing ourselves in the system  $(x, y, z)$  with respect to which the particle has the velocity  $\beta c$  along the  $z$ -axis. The essential point is to determine what will be the form of the wave associated with the particle in the system  $(x, y, z)$ . In the proper system the phase factor was  $\cos 2\pi\nu_0 t_0$ , so that according to the last of

equations (3) in the system  $(x, y, z)$  it will be  $\cos 2\pi\nu_0 \frac{t - \frac{\beta}{c}z}{\sqrt{1 - \beta^2}}$ .

Let us write :

$$\nu = \frac{\nu_0}{\sqrt{1 - \beta^2}}, \quad V = \frac{c}{\beta} = \frac{c^2}{v}, \quad (4)$$

so that the phase factor is  $\cos 2\pi\nu\left(t - \frac{z}{V}\right)$ . The wave will thus appear to the observer of the system  $(x, y, z)$  as a wave of frequency  $\nu$  propagated along the axis of  $z$  with phase velocity  $V$ . This appears as a simple direct consequence of the way in which the time variable is transformed according to the theory of relativity in passing from one Galilean system to another.

The phase velocity of the wave associated with the particle is inversely proportional to the velocity of the particle itself; it is infinite in the proper system where the particle velocity is zero. We have already remarked that according to the dynamics of relativity a particle can never be made to move with a velocity greater than that of light; we have always:

$$\beta < 1, \quad V > c. \quad . \quad . \quad . \quad (5)$$

The sign of equality cannot apply except when the mass is zero, which is the case when the particles are light corpuscles. We shall return to this point later.

## 2. An Alternative Method of Obtaining the Preceding Results

The foregoing results with regard to the phase of the associated wave may also be obtained by the use of a rather more concrete method which gives precision to certain points.

Since the wave has by hypothesis the same frequency and phase at each point of the proper system, we can represent the phase distribution by imagining that synchronous clocks of period,  $T_0 = \frac{1}{\nu_0}$ , are situated at all points of the system. In the system  $(x, y, z)$  each of these clocks will be moving with velocity  $\beta c$ , and will be subject to the relativity retardation. This retardation arises because the clock has a co-ordinate  $z_0$  fixed in the proper system, but in the system  $(x, y, z)$  its  $z$  co-ordinate increases by  $vt$  in time  $t$ . Thus the variation of  $t_0$  recorded by the clock is connected with the variation of  $t$  by the fourth of Lorentz's formulæ:

$$\delta t_0 = \frac{\delta t - \frac{\beta}{c}\delta z}{\sqrt{1-\beta^2}} = \frac{\delta t(1-\beta^2)}{\sqrt{1-\beta^2}} = \delta t\sqrt{1-\beta^2}. \quad . \quad (6)$$



When the clock has completed an oscillation, the lapse of time is  $\delta t_0 = T_0$  in the proper system, and consequently in the system  $(x, y, z)$  the interval is measured by :

$$T_1 = \frac{T_0}{\sqrt{1 - \beta^2}} > T_0. \quad . \quad . \quad . \quad (7)$$

The observer in the latter system attributes to the clock a longer period than that recorded by an observer in the system bound to the clock. This explains the relativity retardation.

Let us pass from periods to frequencies. Each clock has a frequency :

$$\nu_1 = \frac{1}{T_1} = \nu_0 \sqrt{1 - \beta^2} < \nu_0, \quad . \quad . \quad . \quad (8)$$

but at the same time it is in motion with velocity  $v$ .

We shall see that in this motion it remains constantly in phase with the wave :

$$\psi = a \cos 2\pi\nu\left(t - \frac{z}{V}\right). \quad . \quad . \quad . \quad (9)$$

To show this, let us suppose that at a certain instant when  $t = t_1$  the clock agrees in phase with the wave  $\psi$ , as judged by an observer in the system  $(x, y, z)$ .

Then :

$$2\pi\nu\left(t_1 - \frac{z_1}{V}\right) = 2\pi\nu_1 t_1, \quad . \quad . \quad . \quad (10)$$

where  $z_1$  is the value of  $z$  at time  $t_1$ . At a later time  $t_2$  the clock occupies the position  $z_2 = z_1 + v(t_2 - t_1)$ , so that the phase of the wave at this point is  $2\pi\nu\left(t_2 - \frac{z_2}{V}\right)$ , while the phase of the clock is  $2\pi\nu_1 t_2$ . In order that the agreement in phase may persist, it is necessary that

$$\nu_1 t_2 = \nu\left(t_2 - \frac{z_2}{V}\right), \quad . \quad . \quad . \quad (11)$$

which by (10) may be written :

$$\begin{aligned} \nu_1(t_2 - t_1) &= \nu(t_2 - t_1) - \frac{\nu}{V}(z_2 - z_1) \\ &= \nu\left(1 - \frac{v}{V}\right)(t_2 - t_1), \quad . \quad . \quad . \quad (12) \end{aligned}$$

or

$$\nu_1 = \nu(1 - \beta^2). \quad . \quad . \quad . \quad (13)$$

But this equation is identically satisfied on account of the definitions of  $\nu$  and  $\nu_1$  in equations (4) and (8).

### 3. Refractive Index. Fundamental Theorem on the Group-Velocity of the $\psi$ -waves

The phase velocity  $V$  may be used to define an index of refraction for the  $\psi$ -waves in the system  $(x, y, z)$ . We define this index by the usual relation :

$$n = \frac{c}{V}, \quad . \quad . \quad . \quad (14)$$

which gives by (4)

$$n = \beta. \quad . \quad . \quad . \quad (15)$$

Thus, by substituting (15) in the first of the formulæ (4)

$$n = \sqrt{1 - \frac{\nu_0^2}{\nu^2}}. \quad . \quad . \quad . \quad (16)$$

This formula may be considered as defining the dispersion of space for the  $\psi$ -waves associated with a particle the nature of which is characterised by the constant  $\nu_0$ . In other words, if we consider the assembly of possible uniform rectilinear motions of the particle in the system  $(x, y, z)$ , the frequency and phase velocity of the associated wave are always connected by the equation (16).

The dispersion formula just established leads to a very important theorem, but before stating it we must consider the meaning of the term "group velocity," which was introduced by Lord Rayleigh in connection with the propagation of waves in a dispersive medium. A plane monochromatic wave of frequency  $\nu$  which is propagated in a certain direction, which we may take along the axis of  $x$ , is represented by the function  $a \cos 2\pi\nu\left(t - \frac{nx}{c}\right)$ , where  $n$  is the refractive index of the medium for the frequency  $\nu$ . Instead of a single plane monochromatic wave, let us consider a very large number of waves of this kind travelling along the axis of  $x$  with frequencies lying in the small range  $\nu - \delta\nu$  to  $\nu + \delta\nu$ ; this is what is called a

group of waves. An element of the group may be represented by :

$$a_{\nu+\epsilon} d\epsilon \cos 2\pi(\nu + \epsilon) \left\{ t - n_{\nu+\epsilon} \frac{x}{c} + b_{\epsilon} \right\}, \quad |\epsilon| \ll \delta\nu,$$

where  $b_{\epsilon}$  is a phase constant. If at a certain instant all the members of the group agree in phase at a certain point there will be a high resultant amplitude at the point. As the medium is dispersive, which means that the phase velocities differ slightly for the various waves of the group, the waves will get out of step with one another during the propagation. We shall, however, show that a point where there is agreement of phase exists, which travels with a velocity in general different from the phase velocity.

Let there be two waves of the group characterised by the values  $\epsilon_1$  and  $\epsilon_2$ . According to our assumption, the two waves agree in phase for a certain value of  $x$  and for a certain value of  $t$ . Let  $x$  and  $t$  change by amounts  $dx$  and  $dt$  respectively, so that the phase of the first wave changes by

$$2\pi(\nu + \epsilon_1) \left( dt - n_{\nu+\epsilon_1} \frac{dx}{c} \right).$$

Since  $\epsilon_1$  is very small, we may write :

$$n_{\nu+\epsilon_1} = n_{\nu} + \frac{dn_{\nu}}{d\nu} \epsilon_1, \quad . \quad . \quad . \quad (17)$$

provided that  $n$  is continuous. Thus if we neglect quantities of the second order the change in phase in the first wave is :

$$2\pi \left\{ (\nu + \epsilon_1) dt - (\nu + \epsilon_1) n_{\nu} \frac{dx}{c} - \nu \epsilon_1 \frac{dn_{\nu}}{d\nu} \cdot \frac{dx}{c} \right\}.$$

There is, of course, a similar expression in  $\epsilon_2$  for the second wave.

The difference of the two phase changes is :

$$2\pi(\epsilon_2 - \epsilon_1) \left( dt - n_{\nu} \frac{dx}{c} \right) - 2\pi(\epsilon_2 - \epsilon_1) \nu \frac{dn_{\nu}}{d\nu} \cdot \frac{dx}{c}. \quad (18)$$

so that if  $dt$  and  $dx$  satisfy the relation :

$$dt = \left( n_{\nu} + \nu \frac{dn_{\nu}}{d\nu} \right) \frac{dx}{c}, \quad . \quad . \quad . \quad (19)$$

the two waves are still in phase.

This equation defines a velocity  $U$  given by :

$$\frac{1}{U} = \left( \frac{dx}{dt} \right)^{-1} = \frac{1}{c} \left( n_\nu + \nu \frac{dn_\nu}{d\nu} \right) = \frac{1}{c} \frac{d}{d\nu} (n_\nu \nu). \quad (20)$$

If we travel along the axis of  $x$  with velocity  $U$ , we see the two waves always in phase. But  $\epsilon_1$  and  $\epsilon_2$  are arbitrary, and our reasoning holds for all pairs of waves in the group. Thus if we travel with velocity  $U$  along the axis all the waves are seen in phase, in other words, the maximum which arises as a consequence of this agreement in phase travels along the axis with velocity  $U$ , which we describe as the group velocity.

We proceed to establish the theorem that the group velocity of the associated waves of a particle is equal to the velocity of the particle.

The equation of dispersion (16) gives,

$$n\nu = \sqrt{\nu^2 - \nu_0^2}, \quad (21)$$

and

$$\frac{d}{d\nu} (n\nu) = \frac{\nu}{\sqrt{\nu^2 - \nu_0^2}} = \frac{1}{n}. \quad (22)$$

Thus, from (15) and (20),

$$U = nc = \beta c. \quad (23)$$

#### 4. Relations Between Wave and Mechanical Quantities

Hitherto we have introduced no relation between the mechanical quantities, mass, momentum and energy, which are characteristic of the particle and the characteristics of the wave, frequency, phase velocity and index of refraction. Yet if we wish the associated waves to be of use to us in the inclusion of quanta, such relations must exist and, in particular, we must expect to find the energy  $W$  of the particle and the frequency  $\nu$  of its associated wave related by the formula :

$$W = h\nu, \quad (24)$$

where  $h$  is Planck's constant, which is a relation which forms the starting point of the quantum theory.

By the theory of relativity the value of the energy of the particle is :

$$W = \frac{mc^2}{\sqrt{1 - \beta^2}} \quad (25)$$

in the system  $(x, y, z)$ . In the proper system its value is

$$W_0 = mc^2, \quad . \quad . \quad . \quad . \quad (26)$$

whence

$$W = \frac{W_0}{\sqrt{1 - \beta^2}}, \quad . \quad . \quad . \quad . \quad (27)$$

This formula, giving the transformation from  $W_0$  to  $W$ , is thus the same as (4) which transforms  $\nu_0$  to  $\nu$ . Since this similarity in the transformations in the Galilean systems exists, we are justified in adopting the relation :

$$W = h\nu \quad . \quad . \quad . \quad . \quad (28)$$

between the energy of the particle and the frequency of the associated wave, where  $h$  is a constant of proportionality, which is naturally taken to be Planck's constant.

We pass to consider the momentum which is a vector tangential to the trajectory, and has the value,

$$p = \frac{m\nu}{\sqrt{1 - \beta^2}}, \quad . \quad . \quad . \quad . \quad (29)$$

in the dynamics of relativity.

From (25) and (29) it appears that the magnitude of this vector is :

$$|p| = \frac{W}{c^2}v. \quad . \quad . \quad . \quad . \quad (30)$$

If we replace  $W$  by  $h\nu$  and  $\frac{c^2}{v}$  by  $V$ , we see that it is possible to describe momentum as a vector in the direction of the phase velocity of magnitude :

$$|p| = \frac{h\nu}{V} = \frac{h\nu}{c}n. \quad . \quad . \quad . \quad . \quad (31)$$

It is of interest to introduce also at this point the wave length,  $\lambda$ , of the associated wave, by writing as usual :

$$\lambda = \frac{V}{\nu}. \quad . \quad . \quad . \quad . \quad (32)$$

Formula (31) gives :

$$|p| = \frac{h}{\lambda}. \quad . \quad . \quad . \quad . \quad (33)$$

### 5. The Principle of Least Action and Fermat's Principle

We may sum up these points by saying that a particle of mass  $m$ , moving in a certain direction with velocity  $v$  ( $=\beta c$ ), must be associated with a wave of frequency  $\nu = \frac{mc^2}{h\sqrt{1-\beta^2}}$ , travelling in the same direction with phase velocity  $V$  ( $=\frac{c^2}{v}$ ). The wave length is :

$$\lambda = \frac{h}{p} = \frac{h\sqrt{1-\beta^2}}{mv},$$

and the group velocity is  $v$ .

When  $\beta^2$  is negligible with respect to unity, as in Newtonian mechanics, it is sufficient to write :

$$\nu = mc^2 + \frac{1}{2}mv^2 \quad \text{and} \quad \lambda = \frac{h}{mv}.$$

We conclude this chapter with the consideration of an important point. In a medium of refractive index  $n$ , the rays in geometrical optics are limited by the condition, which is Fermat's principle, that the ray which passes through two points A and B must have a form such that the line integral

$$\int_A^B \frac{\nu}{V} dl = \frac{\nu}{c} \int_A^B n dl$$

is a minimum. In our case the index is constant in space and the principle states that the ray joining A and B is a curve of minimum length or a straight line. The rays are rectilinear and the waves are plane. The important point is that,  $\frac{\nu}{V}$  being equal to  $\frac{p}{h}$ , the Fermat integral may be written

$$\frac{1}{h} \int p dl = \frac{1}{h} \int (p_x dx + p_y dy + p_z dz)$$

and it is thus identical with the principle of Maupertuis, except for the constant  $\frac{1}{h}$ . An analogy between this principle for the particle and Fermat's principle for the associated waves thus

appears. We have, in this chapter, established the connection between waves and particles only in the very simple case where there is no field of force. It will be necessary to seek a generalisation of this connection in the case when the particle moves in a field of force. In order to attain this goal we shall rely upon the analogy which we have just pointed out, and this makes it necessary to study rather more closely the question of wave propagation.

## CHAPTER IV

### GENERAL REMARKS ON WAVE PROPAGATION

#### 1. The Propagation of Waves in a Permanent Homogeneous Medium

WE will first consider the simplest case ; that of wave propagation in a space which is homogeneous and has permanent properties. This is the familiar case, for example, of the propagation of light waves in a homogeneous refracting medium. The conditions of propagation are then characterised by a certain quantity, the refractive index  $n$ , constant in space and time. If the velocity of light in empty space is denoted by the constant  $c$  ( $= 3 \times 10^{10}$  cms. per sec.) the wave equation has most frequently the well-known form :

$$\nabla^2 \psi = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{n^2}{c^2} \frac{\partial^2 \psi}{\partial t^2}. \quad (1)$$

A solution of this equation in the form :

$$\psi(x, y, z, t) = a \cos 2\pi \left\{ \nu t - \frac{n\nu}{c} (\alpha x + \beta y + \gamma z) \right\} \quad (2)$$

will be said to represent a simple sinusoidal or plane monochromatic wave.

The constants  $a$  and  $\nu$  are respectively the amplitude and frequency of the wave,  $\alpha, \beta, \gamma$  are direction cosines, and satisfy the relation

$$\alpha^2 + \beta^2 + \gamma^2 = 1.$$

The phase of the plane monochromatic wave is defined by :

$$\Phi(x, y, z, t) = \nu t - \frac{n\nu}{c} (\alpha x + \beta y + \gamma z). \quad (3)$$



It is easy to verify that (2) is a solution of (1). In the first place,  $\frac{\partial^2 \psi}{\partial t^2} = -4\pi^2\nu^2\psi$ , so that we can write (1) in the form :

$$\nabla^2\psi + \frac{4\pi^2n^2\nu^2}{c^2}\psi = 0. \quad . \quad . \quad (4)$$

Moreover,

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2n^2\nu^2}{c^2}\alpha^2\psi, \quad . \quad . \quad (5)$$

and similarly for  $y$  and  $z$ , so that equation (4) is immediately verified on account of the direction cosine relation.

We shall write :

$$\Phi_1(x, y, z, t) = \frac{n\nu}{c}(\alpha x + \beta y + \gamma z). \quad . \quad . \quad (6)$$

At a particular instant the phase (3) will be constant on the planes :

$$\Phi_1 = \text{constant or } \alpha x + \beta y + \gamma z = \text{constant}.$$

These are planes of constant phase, and the quantities  $(\alpha, \beta, \gamma)$  are the direction cosines of the normals to these planes.

As the time passes, the values of the phase  $\Phi$  progress in space, passing from one equiphase plane to another. We may say that the phase travels in the direction  $(\alpha, \beta, \gamma)$  which we call the direction of wave propagation. The parallel straight lines with direction cosines  $(\alpha, \beta, \gamma)$  are the rays, and we can easily calculate the phase velocity, that is the velocity with which it is necessary to travel along the ray to keep up with a certain phase value. Let  $dl$  denote the element of length along the ray, so that :

$$dl = \alpha dx + \beta dy + \gamma dz \quad . \quad . \quad (7)$$

and the change in phase for the given values of  $dt$  and  $dl$  is thus :

$$d\Phi = \nu dt - \frac{n\nu}{c}dl. \quad . \quad . \quad (8)$$

This variation will be zero if we travel along the ray with velocity

$$V = \frac{dl}{dt} = \frac{c}{n}. \quad . \quad . \quad (9)$$

$V$  is the phase velocity.

The wave-length  $\lambda$  is defined in a similar way ; it is the length which must be traversed along the ray at a particular instant in order to obtain a variation in  $\Phi$  of amount unity, which restores to  $\psi$  its original value. We find at once :

$$\lambda = \frac{c}{n\nu} = \frac{V}{\nu}. \quad . \quad . \quad . \quad . \quad (10)$$

## 2. Dispersion

In the foregoing discussion we have supposed  $n$  constant, but it is often necessary to consider  $n$  as a function of  $\nu$  in equation (4), that is to say, that  $n$ , although independent of  $x, y, z$  and  $t$ , is a function of the frequency of the simple sinusoidal wave considered. We say, then, that there is dispersion and the relation between  $n$  and  $\nu$  is called the dispersion formula. In a special case, this occurs when the wave equation in its general form has, instead of (1), the form :

$$\nabla^2\psi - \frac{1}{c^2} \frac{\partial^2\psi}{\partial t^2} = K\psi, \quad . \quad . \quad . \quad (11)$$

where  $K$  is a constant, for then, on substitution of (2), we can write (11) in the form :

$$\nabla^2\psi + \left( \frac{4\pi^2\nu^2}{c^2} - K \right) \psi = 0, \quad . \quad . \quad (12)$$

and to obtain (4) we must write :

$$n^2 = 1 - \frac{Kc^2}{4\pi^2\nu^2} = f(\nu), \quad . \quad . \quad . \quad (13)$$

so that  $n$  depends upon  $\nu$ .

## 3. Trains and Groups of Waves

The plane monochromatic wave must in a certain sense be considered as an abstraction, for it would fill the whole of space and last throughout all time. In practice a wave always occupies a limited region of space at a particular instant, and at any particular point it has a beginning and an end. A wave thus limited is known as a wave train.

To represent a wave train we consider not merely a single

plane monochromatic wave but an assembly of such waves, representing the assembly by :

$$\psi(x, y, z, t) = \sum a(\nu, \alpha, \beta, \gamma) \cos 2\pi \left\{ \nu t - \frac{n}{c} \nu (\alpha x + \beta y + \gamma z) + \Delta(\nu, \alpha, \beta, \gamma) \right\}, \quad (14)$$

where  $\Delta$  denotes that the individual plane monochromatic waves have, in general, different phases. If  $\alpha, \beta, \gamma$  are always related by the equation  $\alpha^2 + \beta^2 + \gamma^2 = 1$ , it follows as above (§ 1) that each individual wave satisfies the wave equation, and on account of the linearity of this equation, the sum of the waves is a solution. Instead of a sum of a finite number of terms we may also consider the integral :

$$\psi(x, y, z, t) = \iiint a(\nu, \alpha, \beta) \cos 2\pi \left\{ \nu t - \frac{n\nu}{c} (\alpha x + \beta y + \gamma z) + \Delta(\nu, \alpha, \beta) \right\} d\nu d\alpha d\beta, \quad (15)$$

with  $\alpha^2 + \beta^2 + \gamma^2 = 1$ .

We must remember that  $n$  may be a function of  $\nu$  in equations (14) and (15). In order to make it clear how one can represent a wave train by a sum of plane monochromatic waves, we shall consider the case of a train travelling along the direction of the  $z$  axis, which may be represented by :

$$\psi(x, y, z, t) = A(x, y, z, t) \cos 2\pi \left( \nu t - \frac{n\nu}{c} z \right), \quad (16)$$

with a suitable choice of the origin of time. We shall suppose, in addition, that the form of the wave train is symmetrical with respect to the  $z$  axis, i.e.  $A$  is an even function of the variables  $x$  and  $y$ .

$$A(-x, y, z, t) = A(x, y, z, t), \quad A(x, -y, z, t) = A(x, y, z, t). \quad (17)$$

Since the wave train is limited in space, at any given time the function  $A$  will be different from zero only if the variables are included between the limits  $(x_1, y_1, z_1)$  and  $(x_2, y_2, z_2)$ . These limits determine the extension of the wave train in space. In order to simplify the analysis a little further we shall suppose that in the region occupied by the wave train at a given instant the value of  $A$  is appreciably constant, except at the boundaries, where it falls rapidly to zero ; in other words,

for given values of  $y$ ,  $z$ , and  $t$  the function  $A$ , considered as a function of  $x$  alone, is zero for  $x < x_1$ , passes rapidly to a constant value in the neighbourhood  $x = x_1$ , remains constant up to  $x = x_2$ , and then falls rapidly to zero (Fig. 1).

The dependence upon  $y$  and  $z$  is of the same type. In short, our wave train may be mistaken in the greatest part of its domain for a plane monochromatic wave, but it differs from it, of course, at the boundaries.

By the definition of a wave group, the assembly of waves constituting it have neighbouring frequencies and directions.

We propose to show that it is possible to represent the wave train studied by means of a group with the condition

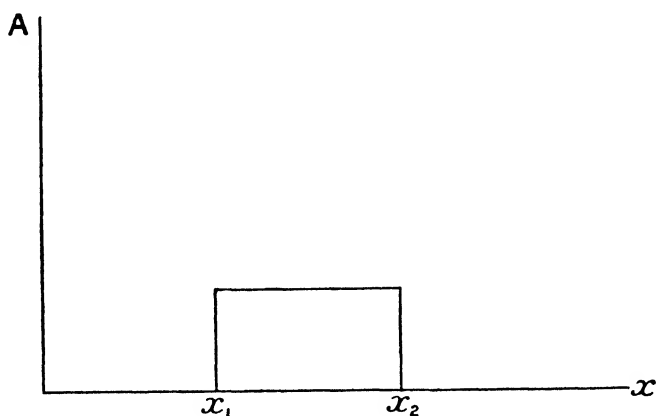


FIG 1.

that the dimensions of the train in space are large in relation to the wave-length, and that its duration at a fixed point is large in relation to the period. On account of the assumed symmetry of the train about the  $z$ -axis, if we represent it by a wave group the form must be :

$$\int_{-\eta_1}^{+\eta_1} d\alpha \int_{-\eta_2}^{+\eta_2} d\beta \int_{-\eta_3}^{+\eta_3} d\epsilon a(\epsilon, \alpha, \beta) \cos 2\pi \left\{ (\nu + \epsilon)t - \frac{(\nu + \epsilon)n_{\nu + \epsilon}}{c} (\alpha x + \beta y + z) + \Delta(\epsilon, \alpha, \beta) \right\}, \quad (18)$$

We have written  $z$  instead of  $\gamma z$ , since  $\alpha$  and  $\beta$  are very small and consequently  $\gamma (= \sqrt{1 - \alpha^2 - \beta^2})$  differs from unity by terms of the second order only.

By limiting ourselves to quantities of the first order, we have :

$$(\nu + \epsilon)n_{\nu+\epsilon} = \nu n + \epsilon \frac{d}{d\nu}(n\nu), \quad (19)$$

and the argument of the cosine in (18) becomes :

$$2\pi \left[ \nu t - \frac{\nu n}{c}(\alpha x + \beta y + z) + \epsilon \left\{ t - \frac{d(n\nu)}{d\nu} \frac{z}{c} \right\} + \Delta(\epsilon, \alpha, \beta) \right]. \quad (20)$$

If we make use of the formula :  $\cos(a + b) = \cos a \cos b - \sin a \sin b$ , we can write (18) in the form :

$$\begin{aligned} & \cos 2\pi \left( \nu t - \frac{\nu n}{c} z \right) \int_{-\eta_1}^{+\eta_1} d\alpha \int_{-\eta_2}^{+\eta_2} d\beta \int_{-\eta_3}^{+\eta_3} d\epsilon a(\epsilon, \alpha, \beta) \\ & \cos 2\pi \left[ \epsilon \left\{ t - \frac{d(n\nu)}{d\nu} \frac{z}{c} \right\} - \frac{\nu n}{c}(\alpha x + \beta y) + \Delta(\epsilon, \alpha, \beta) \right] \\ & - \sin 2\pi \left( \nu t - \frac{\nu n}{c} z \right) \int_{-\eta_1}^{+\eta_1} d\alpha \int_{-\eta_2}^{+\eta_2} d\beta \int_{-\eta_3}^{+\eta_3} d\epsilon a(\epsilon, \alpha, \beta) \\ & \sin 2\pi \left[ \epsilon \left\{ t - \frac{d(n\nu)}{d\nu} \frac{z}{c} \right\} - \frac{\nu n}{c}(\alpha x + \beta y) + \Delta(\epsilon, \alpha, \beta) \right]. \quad (21) \end{aligned}$$

In order to identify this expression for the wave group with (16) for the wave train, it is necessary, in the first place, to make the coefficient in the sine term vanish. To bring this about we shall suppose that  $\Delta$  has the same value for all the monochromatic waves of the group, and we shall then write  $\Delta = 0$ . In addition, we shall suppose that  $a(\epsilon, \alpha, \beta)$  is an even function in the three arguments  $\epsilon, \alpha, \beta$ . This assumption with regard to  $\alpha$  and  $\beta$  corresponds to the symmetry of the wave train about the  $z$ -axis, and with regard to  $\epsilon$  to a symmetry of spectral distribution in the group about the central frequency  $\nu$ .

To complete the identification, it is sufficient to write :

$$\begin{aligned} A(x, y, z, t) &= \int_{-\eta_1}^{+\eta_1} d\alpha \int_{-\eta_2}^{+\eta_2} d\beta \int_{-\eta_3}^{+\eta_3} d\epsilon a(\epsilon, \alpha, \beta) \\ & \cos 2\pi \left[ \epsilon \left\{ t - \frac{d(n\nu)}{d\nu} \frac{z}{c} \right\} - \frac{\nu n}{c}(\alpha x + \beta y) + \Delta(\epsilon, \alpha, \beta) \right]. \quad (22) \end{aligned}$$

The expression (22), when it is exact, that is to say, when the wave train can be exactly represented by a wave group, allows us to determine once more Rayleigh's group velocity.

Let us consider a straight line parallel to the direction of

the  $z$ -axis. When this line is displaced by an amount  $dz$  the displacement is associated with a constant value of  $A$  if it takes a time  $dt = \frac{1}{c} \frac{d(n\nu)}{d\nu} dz$ , to make the displacement. We can thus consider, to the degree of approximation employed<sup>1</sup> that the amplitude resulting from the wave train is displaced in the direction  $z$  with velocity  $U$  defined by the formula :

$$\frac{1}{U} = \frac{1}{c} \frac{d(n\nu)}{d\nu}. \quad . \quad . \quad . \quad (23)$$

This is the group velocity previously introduced. If  $n$  is independent of  $\nu$  we have :  $U = \frac{c}{n}$ , or the group velocity is identical with the phase velocity.

Thus, when (22) is applicable,  $A$  depends upon  $z$  and  $t$  through  $\left(t - \frac{z}{U}\right)$  only, and it is natural to introduce  $z' = z - Ut$ . For any given value of  $t$ ,  $z'$  measures the value of  $z$ , except for a constant, and if  $z_1'$  and  $z_2'$  correspond to points at the beginning and end of the wave train :

$$z_1' - z_2' = z_1 - z_2. \quad . \quad . \quad . \quad (24)$$

It is easy to see that the group (22) is symmetrical in  $z'$  as in  $x$  and  $y$ . We can now write (22) in the form :

$$A(x, y, z') = \int_{-\eta_1}^{+\eta_1} d\alpha \int_{-\eta_2}^{+\eta_2} d\beta \int_{-\eta_3}^{+\eta_3} d\epsilon a(\epsilon, \alpha, \beta) \cos 2\pi \left\{ -\frac{\epsilon}{U} z' - \frac{n\nu}{c} (\alpha x + \beta y) \right\}. \quad (25)$$

If we decompose the integral into a sum of products of sines and cosines, the only part which does not vanish will be that which contains the product of three cosines on account of the evenness of  $a(\epsilon, \alpha, \beta)$ .

Thus if we write :

$$c(\epsilon, \alpha, \beta) = 8a(\epsilon, \alpha, \beta) \quad . \quad . \quad . \quad (26)$$

<sup>1</sup> Actually for intervals of sufficiently long duration a wave train has always a tendency to spread. More rigorous calculations made in Chap. XIII will show this clearly.

we obtain :

$$A(x, y, z') = \int_0^{\eta_1} d\alpha \int_0^{\eta_2} d\beta \int_0^{\eta_3} d\epsilon c(\epsilon, \alpha, \beta) \cos \frac{2\pi\epsilon}{U} z' \cos 2\pi \frac{n\nu}{c} \alpha x \cos 2\pi \frac{n\nu}{c} \beta y. \quad (27)$$

This is the form which  $A$  must take in order that the wave train may be represented by a wave group. But the question arises with regard to the possibility of expressing  $A$  in this way.

Fourier's theory of integrals shows that under very general conditions a function  $f(x, y, z)$ , which is even in  $x, y, z$ , can be expressed in the form :

$$f(x, y, z) = \int_0^\infty d\lambda \int_0^\infty d\mu \int_0^\infty d\nu p(\lambda, \mu, \nu) \cos \lambda x \cos \mu y \cos \nu z, \quad (28)$$

where

$$p(\lambda, \mu, \nu) = \frac{1}{\pi^3} \int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dz f(x, y, z) \cos \lambda x \cos \mu y \cos \nu z. \quad (29)$$

Thus the function  $A(x, y, z')$ , which is even in  $x, y, z'$ , may be written :

$$A(x, y, z') = \int_0^\infty d\alpha \int_0^\infty d\beta \int_0^\infty d\epsilon c(\epsilon, \alpha, \beta) \cos \frac{2\pi\epsilon}{U} z' \cos 2\pi \frac{n\nu}{c} \alpha x \cos 2\pi \frac{n\nu}{c} \beta y, \quad (30)$$

where

$$c(\epsilon, \alpha, \beta) = 8 \int_{-\infty}^\infty \frac{dz'}{U} \int_{-\infty}^\infty \frac{n\nu}{c} dx \int_{-\infty}^\infty \frac{n\nu}{c} dy A(x, y, z') \cos \frac{2\pi\epsilon}{U} z' \cos 2\pi \frac{n\nu}{c} \alpha x \cos 2\pi \frac{n\nu}{c} \beta y. \quad (31)$$

But to be able to represent our wave train by a wave group we must identify (27) and (30), i.e. we must reduce the intervals of integration in (30) to the very small intervals 0 to  $\eta_1$ , 0 to  $\eta_2$ , 0 to  $\eta_3$ . Thus it is necessary that the function  $c(\epsilon, \alpha, \beta)$  defined by (31) should vanish outside these small intervals. Now, by hypothesis,  $A$  is appreciably constant for  $x_1 < x < x_2$ ,  $y_1 < y < y_2$ ,  $z_1 < z < z_2$ , and is zero elsewhere. If in (31) we consider the integral with respect to  $x$ , we have :

$$c(\epsilon, \alpha, \beta) = \text{constant} \times \int_{x_1}^{x_2} A \cos 2\pi \frac{n\nu}{c} \alpha x dx, \quad (32)$$

where  $A$  is appreciably constant. When the cosine has a large number of periods in the region  $x_1$  to  $x_2$ ,  $c(\epsilon, \alpha, \beta)$  is approximately zero. In order that  $c$  may have an appreciable value it is necessary that :

$$\frac{\alpha}{\lambda}(x_1 - x_2) \sim 1, \quad . \quad . \quad . \quad (33)$$

where the sign  $\sim$  denotes "is of the order." In order that this should be equivalent to  $\alpha \ll 1$  it is necessary that :

$$\lambda \ll x_1 - x_2. \quad . \quad . \quad . \quad (34)$$

The dimension of the wave train in the  $x$  direction must be much greater than the average wave-length  $\lambda$ . We find the same result for the  $y$  direction.

For the  $z$  direction we find :

$$\frac{\epsilon}{U}(z_1' - z_2') = \frac{\epsilon}{U}(z_1 - z_2) \sim 1, \quad . \quad . \quad (35)$$

and in order that  $\epsilon \ll \nu$  we require :

$$z_1 - z_2 \gg \frac{U}{\nu} = UT. \quad . \quad . \quad . \quad (36)$$

The product  $UT$  is not, in general, equal to the wave-length  $VT$ , but the two quantities are often of the same order. We can thus say that the wave train can be represented by a group when all its dimensions are great with respect to the wave-length. The time taken by the wave train to pass a fixed point completely is clearly :

$$t_1 - t_2 = \frac{z_1 - z_2}{U}. \quad . \quad . \quad . \quad (37)$$

According to (36) this interval must be long with respect to the period. According to (33), to the similar relation for  $y$  and to (35) the quantities  $\frac{\eta_1}{\lambda}(x_1 - x_2)$ ,  $\frac{\eta_2}{\lambda}(y_1 - y_2)$ , and  $\frac{\eta_3}{U}(z_1 - z_2)$  must be at least of the order unity. Let us describe a vector  $\mathbf{N}$  for a plane monochromatic wave in the direction of propagation and of magnitude equal to the number of waves per cm. by the term "vector wave number." Its components are :

$$N_x = \frac{\alpha}{\lambda}, \quad N_y = \frac{\beta}{\lambda}, \quad N_z = \frac{\gamma}{\lambda}. \quad . \quad . \quad (38)$$



On account of the hypotheses made with regard to  $\alpha$ ,  $\beta$  and  $\gamma$ , the maximum variations of  $N_x$ ,  $N_y$  and  $N_z$  corresponding to the various monochromatic components of the wave train are :

$$\delta N_x = \frac{\eta_1}{\lambda}, \quad \delta N_y = \frac{\eta_2}{\lambda}, \quad \delta N_z = \delta\left(\frac{1}{\lambda}\right) = \frac{\partial\left(\frac{1}{\lambda}\right)}{\partial\nu} \eta_3 = \frac{\eta_3}{U}. \quad (39)$$

Let us write :

$$\delta x = x_1 - x_2, \quad \delta y = y_1 - y_2, \quad \delta z = z_1 - z_2. \quad (40)$$

These are the maximum variations of the co-ordinates throughout the extent of the wave train. We may therefore write the inequalities in order of magnitude :

$$\delta N_x \cdot \delta x \gg 1, \quad \delta N_y \cdot \delta y \gg 1, \quad \delta N_z \cdot \delta z \gg 1. \quad (41)$$

Finally, let us write :

$$\delta t = t_1 - t_2 \quad . \quad . \quad . \quad . \quad (42)$$

for the time of passage of the wave train at a fixed point, and  $\delta\nu$  for the maximum variation in frequency in the group, so that by (35) and (37)

$$\delta\nu \cdot \delta t \gg 1. \quad . \quad . \quad . \quad . \quad (43)$$

We shall see later the importance of (41) and (43) in the theory of Bohr and Heisenberg.

#### 4. Propagation in a Permanent Heterogeneous Medium

Hitherto we have assumed that the index of refraction was independent of  $x$ ,  $y$  and  $z$ . We will now suppose it a function of these variables, but independent of the time. This is the case occurring in optics for refracting, heterogeneous media. In general, the index depends upon the frequency or heterogeneous refracting media are dispersive.

The equation of propagation of simple sinusoidal waves will in this case be :

$$\nabla^2\psi + \frac{4\pi^2\nu^2 n^2}{c^2}\psi = 0, \quad . \quad . \quad . \quad (44)$$

where  $n$  is now a function of  $x$ ,  $y$ ,  $z$ .

Let us consider the sinusoidal solution :

$$\psi = a(x, y, z) \cos 2\pi\{vt - \Phi_1(x, y, z)\}, \quad (45)$$

where  $a$  is the amplitude and is variable from point to point.

The quantity

$$\Phi(x, y, z, t) = vt - \Phi_1(x, y, z) \quad (46)$$

is the phase, and is still linear in  $t$ , though no longer linear in  $x, y, z$ .

If we substitute (45) in (44) we obtain :

$$\left\{ \nabla^2 a - 4\pi^2 a \sum \left( \frac{\partial \Phi_1}{\partial x} \right)^2 + \frac{4\pi^2 \nu^2}{c^2} n^2 a \right\} \cos 2\pi(vt - \Phi_1) \\ + \left( 4\pi \sum \frac{\partial \Phi_1}{\partial x} \cdot \frac{\partial a}{\partial x} + 2\pi a \nabla^2 \Phi_1 \right) \sin 2\pi(vt - \Phi_1) = 0. \quad (47)$$

Since this equation must be always satisfied, the coefficients of the sine and cosine terms are each equal to zero, so that :

$$\sum \left( \frac{\partial \Phi_1}{\partial x} \right)^2 = \frac{n^2 \nu^2}{c^2} + \frac{1}{4\pi^2} \frac{\nabla^2 a}{a} \quad (48)$$

$$\sum \frac{\partial \Phi_1}{\partial x} \frac{\partial a}{\partial x} + \frac{1}{2} a \nabla^2 \Phi_1 = 0. \quad (49)$$

We shall describe as the wave-length the quantity  $\lambda$  where :

$$\frac{1}{\lambda} = \frac{\partial \Phi_1}{\partial l}, \quad (50)$$

where  $dl$  denotes an element of length along the normal to the surface,  $\Phi_1 = \text{constant}$ , at the point under consideration. In this case,  $\lambda$  varies from point to point.

This definition, of course, includes the case where  $n$  is constant, for then the surfaces,  $\Phi_1 = \frac{n\nu}{c}(\alpha x + \beta y + \gamma z) = \text{constant}$ , are planes of which the normal has direction cosines  $(\alpha, \beta, \gamma)$  and

$$\frac{\partial \Phi_1}{\partial l} = \frac{n\nu}{c} = \frac{\nu}{V}.$$

As in the case of homogeneous media, we shall describe the surfaces,  $\Phi_1 = \text{constant}$ , as surfaces of constant phase, and these are not, in general, plane. The curves normal to these surfaces are still called rays, and we shall call the velocity with

which it is necessary to move along a ray to accompany a constant value of the phase the phase velocity  $V(x, y, z)$ .

It is easy to determine  $V$ , for if we traverse a length  $dl$  of the ray in time  $dt$  the change in  $\Phi_1$  is  $\left(\nu dt - \frac{\partial \Phi_1}{\partial l} dl\right)$ , and for this to be zero we must have :

$$V = \frac{dl}{dt} = \frac{\nu}{\frac{\partial \Phi_1}{\partial l}} = \nu \div \sqrt{\sum \left(\frac{\partial \Phi_1}{\partial x}\right)^2} = \nu \lambda. \quad (51)$$

The function (45) can thus be written in the form :

$$\psi = a(x, y, z) \cos 2\pi \left( \nu t - \nu \int \frac{dl}{V} \right), \quad (52)$$

the integral being taken along the ray to the particular point  $M(x, y, z)$  from a certain surface of constant phase chosen as origin. But, in general, the function  $V(x, y, z)$  is not known *a priori* and its determination requires the evaluation of  $a(x, y, z)$  and  $\Phi_1(x, y, z)$  by means of the simultaneous partial differential equations (48) and (49).

Nevertheless, there is a very interesting case where the determination of  $V$  and of  $\Phi_1$  can be carried out at once without a determination of  $a$ . This is the case in which the medium may be considered homogeneous and the refractive index constant for variations of the order of the wave-length. We shall then have :

$$\left. \begin{aligned} \frac{\partial a}{\partial x} \lambda \ll a, \quad \frac{\partial^2 a}{\partial x^2} \lambda^2 \ll a, \\ \text{with similar relations for } y \text{ and } z, \text{ and :} \\ \lambda^2 \cdot \nabla^2 a \ll a \end{aligned} \right\} \quad (53)$$

The last of these equations taken with the definition of  $\lambda$  in (50) shows that in (48) the term  $\frac{1}{4\pi^2} \frac{\nabla^2 a}{a}$  is negligible with respect to  $\sum \left(\frac{\partial \Phi_1}{\partial x}\right)^2$ , since this is equal to  $\frac{1}{\lambda^2}$ . Moreover, by multiplication of (49) by  $\lambda^2$ , and making use of (50), we find :

$$\frac{1}{a} \frac{\partial a}{\partial l} \lambda + \frac{1}{2} \lambda^2 \nabla^2 \Phi_1 = 0, \quad (54)$$

and by (53) the first term may be neglected.

Finally, (48) and (49) may be written :

$$\left(\frac{\partial \Phi_1}{\partial l}\right)^2 = \frac{n^2 \nu^2}{c^2}, \quad \lambda^2 \nabla^2 \Phi_1 = 0. \quad (55)$$

We will write in agreement with (51) :

$$V = \frac{\nu}{\frac{\partial \Phi_1}{\partial l}} = \frac{c}{n}, \quad \lambda = \frac{V}{\nu} = \frac{c}{n\nu}. \quad (56)$$

The second equation (55) is necessarily true, since  $\Phi_1$  is appreciably linear in  $(x, y, z)$  in measurements of the order of the wave-lengths, and thus quantities such as  $\sum \frac{\partial^2 \Phi_1}{\partial x^2} \cdot \lambda^2$  are negligible.

Formula (52) therefore gives in this case the approximate solution :

$$\psi(x, y, z, t) = a(x, y, z) \cos 2\pi \left( \nu t - \nu \int \frac{ndl}{c} \right), \quad (57)$$

and the determination of  $\Phi_1$  is made *a priori*, since  $n$  is given, without the necessity of calculating  $a$ .

When the foregoing approximation is satisfactory we say that geometrical optics is applicable. We can thus say that for an extension of the order of magnitude of a wave-length the wave is plane and monochromatic, but for an extension containing many wave-lengths there is a progressive variation in the conditions of propagation appearing as a variation in amplitude and a non-linear form of the phase.

## 5. Construction of Wave Envelopes and Fermat's Principle

We suppose that the conditions are such that geometrical optics is applicable and pass on to study the propagation of a wave. If we know one surface of constant phase we can construct others infinitely close to it by describing about each point  $M$  of it a sphere of radius  $\epsilon V_M$ , where  $\epsilon$  is an infinitely small constant and where  $V_M$  is the value of  $V$  at the point  $M$ . The two sheets of the envelope of these small spheres are surfaces of constant phase, for they are surfaces on which at the times  $(t - \epsilon)$  and  $(t + \epsilon)$  we find the value of the phase which at time  $t$  is associated with the known surface. The

two straight lines which join each point M to the points of contact of the sphere of which it is the centre with the envelope are elements of rays. By proceeding in this way, step by step, we can construct all the constant phase surfaces and at the same time we determine the rays as limits of broken lines.

This method, known as the construction of wave envelopes, makes it possible to demonstrate Fermat's principle, which, in geometrical optics, is a postulate. According to this principle any ray passing through two points A and B is such that the line integral

$$\int_A^B \frac{dl}{V} = \int_A^B \frac{n dl}{c}, \quad . \quad . \quad . \quad . \quad (58)$$

taken along the ray, has a stationary value. From the point of view of the wave this means that the time taken by the phase to go from A to B is a minimum along the ray.

To prove this let  $\Phi_1(x, y, z) = C_1$  and  $\Phi_1(x, y, z) = C_2$  be two constant phase surfaces through A and B respectively. Let the intermediate constant phase surfaces be represented by  $\Phi_1(x, y, z) = C$ , where C may have a series of infinitely close values between  $C_1$  and  $C_2$ . The ray from A to B may be regarded as formed of small straight segments normal to this series of surfaces. Any varied curve infinitely close to the ray is formed of infinitely small straight lines having the character just described and of at least two segments not normal to the equiphase surfaces which pass through their extremities. The quantity  $\frac{dl}{V}$  taken over the normal elements is equal to this quantity taken along a ray, for since the elements in each case are normal to surfaces  $\Phi_1 = C$  and  $\Phi_1 = C + dC$  passing through their extremities, we have for each :

$$\frac{dl}{V} = \frac{1}{v} \frac{\partial \Phi_1}{\partial l} \cdot dl = \frac{dC}{v}.$$

If we compare a non-normal element of the varied curve with the corresponding element of the ray, the quantity  $\frac{dl}{V}$  is greater

for the former than for the latter, since the perpendicular is shorter than the oblique element. This proves the principle which is no longer a postulate but a theorem, valid, however, only when we can apply the principles of geometrical optics.

### 6. Wave Groups in a Permanent Heterogeneous Medium

We must now enquire how the conception of wave groups can be generalised in the case of permanent heterogeneous media when geometrical optics may be applied. The function  $\Phi_1$  then satisfies the equation :

$$\left(\frac{\partial \Phi_1}{\partial x}\right)^2 + \left(\frac{\partial \Phi_1}{\partial y}\right)^2 + \left(\frac{\partial \Phi_1}{\partial z}\right)^2 = \frac{\nu^2}{V^2} = \frac{n^2 \nu^2}{c^2}, \quad (59)$$

which is often described as the equation of geometrical optics.

The equiphase surface which serves as the starting point in the construction of the wave envelopes is one of a family of complete integrals :

$$\Phi_1(x, y, z, a, b) = \text{constant}, \quad (60)$$

of equation (59), and the surfaces obtained by this construction belong to this family, the constant alone varying as we pass from one member of the family to another. Thus for a definite propagation the equiphase surfaces form a family with two parameters. In the special case of homogeneous media, we have :  $\Phi_1 = \frac{n\nu}{c}(\alpha x + \beta y + \gamma z)$ , the two parameters  $a$  and  $b$  being the direction cosines  $\alpha$  and  $\beta$ , where we still take  $\gamma = \sqrt{1 - \alpha^2 - \beta^2}$ .

Let us consider a group of waves consisting of an infinity of simple sine waves with frequencies comprised within the small interval  $(\nu - \delta\nu)$  to  $(\nu + \delta\nu)$  for which the parameters  $a$  and  $b$  have values in the small intervals  $(a - \delta a)$ ,  $(a + \delta a)$  and  $(b - \delta b)$ ,  $(b + \delta b)$ , and let us suppose that all the waves are in phase at the point  $(x_0, y_0, z_0)$ . We enquire how this state of phase agreement will be displaced. The function  $\Phi_1$  depending upon  $V$  depends in general upon  $\nu$ , and in order that the waves of the group may be all in phase at the instant  $t_0$ , at the point  $(x_0, y_0, z_0)$ , it is necessary that :

$$t_0 d\nu - \left\{ \left(\frac{\partial \Phi_1}{\partial a}\right)_0 da + \left(\frac{\partial \Phi_1}{\partial b}\right)_0 db + \left(\frac{\partial \Phi_1}{\partial \nu}\right)_0 d\nu \right\} = 0, \quad (61)$$

where the suffix 0 denotes that the values are those at  $(x_0, y_0, z_0)$  and where  $da, db, d\nu$  have values less than  $\delta a, \delta b, \delta \nu$ . If this

agreement in phase is to be found at a later time  $t$  at a point  $(x, y, z)$  we require :

$$td\nu - \left( \frac{\partial \Phi_1}{\partial a} da + \frac{\partial \Phi_1}{\partial b} db + \frac{\partial \Phi_1}{\partial \nu} d\nu \right) = 0, \quad (62)$$

where the derivatives have the values at  $(x, y, z)$  and the same limits are imposed upon  $da$ ,  $db$ , and  $d\nu$ .

The relation (62) will follow from (61) if we have :

$$\frac{\partial \Phi_1}{\partial a} = C_1, \quad \frac{\partial \Phi_1}{\partial b} = C_2, \quad \frac{\partial \Phi_1}{\partial \nu} - t = C_3. \quad (63)$$

The first two relations give the locus of the point where this phase agreement exists, and the third describes the motion of the point on its trajectory. The analogy with Jacobi's theory is obvious.

It is easy to show that the locus obtained in this way is normal to the equiphase surfaces. For by differentiation :

$$\frac{\partial^2 \Phi_1}{\partial x \partial a} dx + \frac{\partial^2 \Phi_1}{\partial y \partial a} dy + \frac{\partial^2 \Phi_1}{\partial z \partial a} dz = 0, \quad (64)$$

$$\frac{\partial^2 \Phi_1}{\partial x \partial b} dx + \frac{\partial^2 \Phi_1}{\partial y \partial b} dy + \frac{\partial^2 \Phi_1}{\partial z \partial b} dz = 0. \quad (64a)$$

By differentiation of equation (59) with respect to  $a$  and  $b$  :

$$\frac{\partial \Phi_1}{\partial x} \cdot \frac{\partial^2 \Phi_1}{\partial a \partial x} + \frac{\partial \Phi_1}{\partial y} \cdot \frac{\partial^2 \Phi_1}{\partial a \partial y} + \frac{\partial \Phi_1}{\partial z} \cdot \frac{\partial^2 \Phi_1}{\partial a \partial z} = 0, \quad (65)$$

$$\frac{\partial \Phi_1}{\partial x} \cdot \frac{\partial^2 \Phi_1}{\partial b \partial x} + \frac{\partial \Phi_1}{\partial y} \cdot \frac{\partial^2 \Phi_1}{\partial b \partial y} + \frac{\partial \Phi_1}{\partial z} \cdot \frac{\partial^2 \Phi_1}{\partial b \partial z} = 0. \quad (65a)$$

If these two systems of equations be compared, it will be seen that :

$$\frac{\partial \Phi_1}{\partial x}, \quad \frac{\partial \Phi_1}{\partial y} \text{ and } \frac{\partial \Phi_1}{\partial z}$$

are proportional respectively to  $dx$ ,  $dy$  and  $dz$  taken along the trajectory. Thus this curve is normal to the surfaces  $\Phi_1 = \text{constant}$ .

When geometrical optics is applicable and the dimensions are of the order of a wave-length, the propagation proceeds as if the refractive index were constant, and even in a region containing a certain number of wave-lengths the waves (45)

may be considered as plane and as having a constant amplitude. But in the cases usually occurring the wave-length is much smaller than the smallest dimensions directly measurable. It will thus be possible to consider wave trains with very small dimensions, as judged by ordinary standards, but which contain a large number of wave-lengths. These trains can be represented by a wave group with neighbouring frequencies and directions which at each instant can be regarded as appreciably plane and as having a constant amplitude, but, of course, the amplitude and phase will be slowly changed during the propagation on account of the large scale variation of the refractive index.

## 7. Propagation of Waves in a Non-Permanent Medium

Finally, we consider the most general case where the conditions of propagation vary not only in space but also in time ; this is the case of heterogeneous, non-permanent refractive media. Let us take, for example, the equation of propagation :

$$\nabla^2 \Psi = \frac{n^2}{c^2} \frac{\partial^2 \Psi}{\partial t^2}, \quad . \quad . \quad . \quad (66)$$

where  $n$  is a function of  $x, y, z$  and  $t$ . Since the time in this equation plays no distinctive part we can no longer eliminate it by taking a sinusoidal solution of which the phase is linear in the time.

We shall thus take for the general form of the sinusoidal solution :

$$\psi(x, y, z, t) = a(x, y, z, t) \cos 2\pi \Phi(x, y, z, t). \quad . \quad (67)$$

If we substitute in equation (66) and equate to zero the coefficients of the sine and cosine terms we obtain :

$$\sum \left( \frac{\partial \Phi}{\partial x} \right)^2 = \frac{n^2}{c^2} \left( \frac{\partial \Phi}{\partial t} \right)^2 + \frac{1}{4\pi^2 a} \left( \nabla^2 a - \frac{n^2}{c^2} \frac{\partial^2 a}{\partial t^2} \right) \quad . \quad (68)$$

$$\sum \frac{\partial \Phi}{\partial x} \frac{\partial a}{\partial x} - \frac{n^2}{c^2} \frac{\partial \Phi}{\partial t} \frac{\partial a}{\partial t} + \frac{a}{2} \left( \nabla^2 \Phi - \frac{n^2}{c^2} \frac{\partial^2 \Phi}{\partial t^2} \right) = 0. \quad . \quad (69)$$

We will write, as a definition of  $\nu$  and  $\lambda$  :

$$\nu(x, y, z, t) = \frac{\partial \Phi}{\partial t}, \quad \lambda(x, y, z, t) = \left( \frac{\partial \Phi}{\partial t} \right)^{-1}, \quad . \quad (70)$$



$dl$  being an element of the normal to  $\Phi = \text{constant}$  at the point and at the instant considered. The frequency and wave-length defined in this way are in general both variable, but when  $n$  is constant they coincide with the frequency and wave-length in the usual sense of these terms. We shall say that the approximation of geometrical optics is valid if the conditions of propagation vary very little over extents in space of the order of  $\lambda$  or over intervals of time of the order of the period  $\frac{1}{\nu}$ . We can then write by (68) :

$$\sum \left( \frac{\partial \Phi}{\partial x} \right)^2 = \frac{n^2}{c^2} \left( \frac{\partial \Phi}{\partial t} \right)^2 \quad . \quad . \quad (71)$$

where we consider the derivatives of the second order as zero.

Equation (71) is the form taken by the equation of geometrical optics (59) which is appropriate to the general case. Over distances of the order of the wave-length, and during intervals which are not very large with respect to the period, we can consider (67) as a plane monochromatic wave. This is the basis of the possibility of imagining in this case trains of waves of which the space and time dimensions are less than those we can measure and which still satisfy the conditions necessary for their representation by a wave group.

Let  $\Phi(x, y, z, t, a, b, c)$  be a complete integral of equation (71), and let a group be formed of sinusoidal waves for which the constants  $a, b$  and  $c$  are included within the limits  $a - \delta a, a + \delta a$ ;  $b - \delta b, b + \delta b$ ;  $c - \delta c, c + \delta c$ .

Let all the waves be supposed in phase at the time  $t_0$  at the point  $(x_0, y_0, z_0)$ , whence :

$$\left( \frac{\partial \Phi}{\partial a} \right)_0 da + \left( \frac{\partial \Phi}{\partial b} \right)_0 db + \left( \frac{\partial \Phi}{\partial c} \right)_0 dc = 0, \quad . \quad (72)$$

where the suffix denotes that the values are appropriate to the chosen time  $t_0$  and the point  $(x_0, y_0, z_0)$ , and where  $da, db, dc$  are less than  $\delta a, \delta b, \delta c$ , respectively. If the agreement in phase recurs again at a point  $(x, y, z)$  at the time  $t$ , we must have :

$$\frac{\partial \Phi}{\partial a} da + \frac{\partial \Phi}{\partial b} db + \frac{\partial \Phi}{\partial c} dc = 0. \quad . \quad . \quad (73)$$

In order that (73) may be a consequence of (72) we require :

$$\frac{\partial \Phi}{\partial a} = C_1, \quad \frac{\partial \Phi}{\partial b} = C_2, \quad \frac{\partial \Phi}{\partial c} = C_3. \quad . \quad . \quad (74)$$

These three equations give the locus of the agreement in phase, and again the analogy with Jacobi's theory is obvious.

Following this study of wave propagation, we pass on to seek the equations of propagation which we must adopt in wave mechanics for the associated waves of a particle.

## CHAPTER V

### THE EQUATIONS OF PROPAGATION OF THE WAVE ASSOCIATED WITH A PARTICLE

#### 1. The Criterion for the Choice of the Equations of Propagation

**I**N the special case of the motion of a particle in the absence of a field of force it has been possible to establish a correspondence between waves and particles. This correspondence finds expression in the statement that a particle of energy  $W$  and of momentum  $\mathbf{p}$  must be associated with a wave travelling in the direction of motion, which is the direction of the vector  $\mathbf{p}$ , and which has the frequency  $\nu \left( = \frac{W}{h} \right)$  and wave-length  $\lambda = \frac{h}{p}$ . The motion proceeds as if empty space had an index of refraction for this wave of value  $n = \sqrt{1 - \frac{\nu^2}{\nu_0^2}}$ , where  $\nu_0$  denotes a constant characteristic of the particle and related to its proper mass  $m$  by the relation  $\nu_0 = \frac{mc^2}{h}$ . The velocity of the particle is equal to the velocity of the group corresponding to this law of dispersion.

Further, there has been revealed (Chap. III, § 5) a connection between the principle of least action and Fermat's principle, and this analogy between the old mechanics and geometrical optics has been confirmed by the fact that the motion of a wave group, when the order of approximation is that of geometrical optics, is expressible by equations strikingly analogous to those of Jacobi (Chap. IV).

We shall thus seek equations of propagation for the associated waves such that, to this order of approximation, the rays coincide with the trajectories of the old dynamics.

One essential point may be mentioned. The wave-length

$\lambda$  and the period  $T (= \frac{1}{\nu})$  of the associated waves are proportional to Planck's constant  $h$ . Now we have seen in the last chapter that when  $\lambda$  and  $T$  become very small the principles of geometrical optics become exactly applicable. Thus whenever it is legitimate to consider  $h$  as a negligible quantity the old mechanics is sufficient. We must choose our wave equations in such a way that when  $h$  tends to zero they give us the equations of the old mechanics. This is a criterion for the choice of the equations.

## 2. The Wave Equation in the Absence of a Field of Force

We take first the simplest case of motion with no field of force. It is agreed that we must adopt the equation :

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \frac{4\pi^2 m^2 c^2}{h^2} \psi. \quad (1)$$

Let us substitute the expression which represents a plane monochromatic wave. Since we have  $\frac{\partial^2 \psi}{\partial t^2} = 4\pi^2 \nu^2 \psi$  in this case, (1) becomes

$$\nabla^2 \psi + \frac{4\pi^2 \nu^2}{c^2} \left(1 - \frac{m^2 c^4}{h^2 \nu^2}\right) \psi = 0. \quad (2)$$

Since  $mc^2 = h\nu_0$ , by definition, we can also write (2) in the form :

$$\nabla^2 \psi + \frac{4\pi^2 \nu^2}{c^2} \left(1 - \frac{\nu_0^2}{\nu^2}\right) \psi = 0. \quad (3)$$

This goes back to the form (4) of the preceding chapter, if we write :

$$n = \sqrt{1 - \frac{\nu_0^2}{\nu^2}}. \quad (4)$$

This is what we ought to find in order to be in agreement with the former results which we have just recalled.

Let us write the simple sinusoidal wave in the form :

$$\psi(x, y, z, t) = a \cos 2\pi \left\{ \nu t - \frac{n\nu}{c} (ax + \beta y + \gamma z) \right\} = a \cos \frac{2\pi}{h} \phi, \quad (5)$$

in which  $\frac{\phi}{h}$  denotes what  $\Phi$  denoted in the preceding chapter, and from this point the term phase will be applied to  $\phi$ .

Thus :

$$\phi = h\nu t - h\nu \frac{n}{c}(\alpha x + \beta y + \gamma z) \quad . \quad . \quad (6)$$

and consequently :

$$\frac{\partial \phi}{\partial t} = h\nu, \quad \frac{\partial \phi}{\partial x} = -\frac{nh\nu}{c} \alpha, \quad \frac{\partial \phi}{\partial y} = -\frac{nh\nu}{c} \beta, \quad \frac{\partial \phi}{\partial z} = -\frac{nh\nu}{c} \gamma. \quad (7)$$

We must write :

$$h\nu = W, \quad \frac{nh\nu}{c} = \frac{h}{\lambda} = p, \quad . \quad . \quad . \quad (8)$$

so that we deduce :

$$W = \frac{\partial \phi}{\partial t}, \quad p_x = -\frac{\partial \phi}{\partial x}, \quad p_y = -\frac{\partial \phi}{\partial y}, \quad p_z = -\frac{\partial \phi}{\partial z}. \quad (9)$$

These are exactly the equations which Jacobi's function satisfies, and we are thus led to identify the phase with this function.

### 3. The Wave Equation in a Constant Field of Force

Let us take the slightly more complicated case of a constant field of force which corresponds to the case of permanent but heterogeneous refracting media. The field of force is characterised by a potential function  $F(x, y, z)$ . The law of dispersion, which, as we shall show, it is convenient to adopt, is :

$$n = \sqrt{\left(1 - \frac{F}{h\nu}\right)^2 - \frac{\nu_0^2}{\nu^2}} \quad . \quad . \quad (10)$$

where  $m c^2 = h\nu_0$ . We obtain, of course, the law of dispersion given by (4) for a zero field of force when  $F = 0$ . The wave equation for monochromatic waves of frequency  $\nu$  must then be written :

$$\nabla^2 \psi + \frac{4\pi^2 \nu^2}{c^2} \left\{ \left(1 - \frac{F}{h\nu}\right)^2 - \frac{\nu_0^2}{\nu^2} \right\} \psi = 0. \quad . \quad (11)$$

From what we know already, geometrical optics will apply if the function  $F(x, y, z)$  varies slowly enough to be considered appreciably constant in a region containing many wave-lengths. We may then take as the solution :

$$\psi(x, y, z, t) = a \cos 2\pi \left( \nu t - \frac{\nu}{c} \int n dl \right), \quad . \quad (12)$$

the integral being taken along a curve normal to a family of complete integrals of the equation :

$$\left(\frac{\partial\Phi_1}{\partial x}\right)^2 + \left(\frac{\partial\Phi_1}{\partial y}\right)^2 + \left(\frac{\partial\Phi_1}{\partial z}\right)^2 = \frac{n^2}{c^2}\nu^2, \quad (13)$$

the integrals depending upon two parameters,  $\alpha$  and  $\beta$ , and  $n$  being a function of  $x$ ,  $y$  and  $z$ .

In a wave group the locus of phase agreement is defined by the equations :

$$\frac{\partial\Phi_1}{\partial\alpha} = C_1, \quad \frac{\partial\Phi_1}{\partial\beta} = C_2$$

and motion on the locus by :

$$\frac{\partial\Phi}{\partial\nu} = t + C_3.$$

In order to arrive at the laws of the old dynamics, it will suffice to suppose that the phase :

$$h\Phi = \phi = h\nu t - \frac{h\nu}{c} \int n dl = h\nu t - \phi_1(x, y, z) \quad (14)$$

is to be identified with Jacobi's function :

$$\begin{aligned} S(x, y, z, t, W, \alpha, \beta) &= Wt - \int (p_x dx + p_y dy + p_z dz) \\ &= Wt - S_1(x, y, z, W, \alpha, \beta). \end{aligned} \quad (15)$$

This leads us to write :

$$\begin{aligned} \frac{\partial\phi}{\partial t} &= \frac{\partial S}{\partial t} = W = h\nu, \\ -\frac{\partial\phi}{\partial x} &= \frac{\partial S_1}{\partial x} = p_x = \frac{nh\nu}{c}\alpha, \end{aligned} \quad (16)$$

with similar equations in  $y$  and  $z$ , whence :

$$p = \frac{nh\nu}{c} = \frac{h\nu}{V} = \frac{h}{\lambda}. \quad (17)$$

From this identification of  $S$  with  $\phi$  and of  $S_1$  with  $\phi_1$  we deduce several important theorems.

*Theorem I.*—The principle of least action of Maupertuis coincides with Fermat's principle.

We have, in fact,

$$\begin{aligned}\int dS_1 &= \int (p_x dx + p_y dy + p_z dz) = \int d\phi_1 \\ &= \int \frac{nh\nu}{c} (\alpha dx + \beta dy + \gamma dz) = \frac{h\nu}{c} \int n dl, \quad (18)\end{aligned}$$

and the condition of Maupertuis,  $\delta S_1 = 0$ , coincides with that of Fermat,  $\delta \int n dl = 0$ .

In other words, the rays of the associated wave are identical with the possible trajectories of the particle which correspond to a complete integral of Jacobi's equation.

*Theorem II.*—The equation of geometrical optics coincides with that of Jacobi.

In its relativistic form the latter is :

$$\frac{1}{c^2} \left( \frac{\partial S}{\partial t} - F \right)^2 - \left( \frac{\partial S}{\partial x} \right)^2 - \left( \frac{\partial S}{\partial y} \right)^2 - \left( \frac{\partial S}{\partial z} \right)^2 = m^2 c^2 \quad (19)$$

and in the present case may be written :

$$\begin{aligned}\frac{1}{c^2} (h\nu - F)^2 - \left( \frac{\partial S_1}{\partial x} \right)^2 - \left( \frac{\partial S_1}{\partial y} \right)^2 - \left( \frac{\partial S_1}{\partial z} \right)^2 &= \frac{h^2 \nu_0^2}{c^2}, \\ \left( \frac{\partial S_1}{\partial x} \right)^2 + \left( \frac{\partial S_1}{\partial y} \right)^2 + \left( \frac{\partial S_1}{\partial z} \right)^2 &= \frac{h^2 \nu^2}{c^2} \left\{ \left( 1 - \frac{F}{h\nu} \right)^2 - \frac{\nu_0^2}{\nu^2} \right\} = \frac{n^2 h^2 \nu^2}{c^2}. \quad (20)\end{aligned}$$

If we replace  $\Phi_1$  by  $\frac{\phi_1}{h} = \frac{S_1}{h}$  in equation (13) we obtain (20), and thus the theorem is proved.

*Theorem III.*—The equations of the trajectory and of motion which are given by the theory of Jacobi are identical with those of the locus and motion of points where there is agreement in phase in a wave group. This is a direct consequence of the relation  $\phi = S$ .

*Theorem IV.*—The velocity of the particle defined by the old dynamics is the same as the group velocity of the associated waves.

To show this directly we start from Jacobi's equation of motion :

$$\frac{\partial S_1}{\partial W} = t + C_3. \quad . \quad . \quad . \quad (21)$$

If  $dl$  is an element of the path described by the particle in time  $dt$ , we have :

$$\frac{\partial^2 S_1}{\partial l \partial W} dl = dt, \quad . \quad . \quad . \quad (22)$$

and since  $\frac{\partial S_1}{\partial l} = p$ , the speed of the particle is given by  $v$ , where :

$$\frac{1}{v} = \left( \frac{dl}{dt} \right)^{-1} = \frac{\partial^2 S_1}{\partial l \partial W} = \frac{\partial p}{\partial W}. \quad . \quad . \quad (23)$$

This may be written :

$$\frac{1}{v} = \frac{\partial p}{\partial W} = \frac{\partial \left( \frac{nh\nu}{c} \right)}{\partial (h\nu)} = \frac{1}{c} \frac{\partial (n\nu)}{\partial \nu} = \frac{1}{U}, \quad . \quad . \quad (24)$$

which is the result required to establish the theorem.

We have seen above that the relativistic form of the wave equation in a constant field of force is given by (11). In the case where Newtonian mechanics is sufficient we may write :

$$h\nu = mc^2 + E = mc^2 + \frac{1}{2}mv^2 + F(x, y, z), \quad . \quad (25)$$

and the quotients  $\frac{E}{h\nu}$  and  $\frac{F}{h\nu}$  are very small in comparison with unity.

We may thus write approximately :

$$\begin{aligned} n &= \sqrt{\left(1 - \frac{F}{h\nu}\right)^2 - \frac{\nu_0^2}{\nu^2}} = \sqrt{1 - \frac{2F}{h\nu} - \left(\frac{h\nu - E}{h\nu}\right)^2} \\ &= \sqrt{\frac{2(E - F)}{h\nu}} = \sqrt{\frac{2(E - F)}{mc^2}}. \end{aligned} \quad (26)$$

This is the law of dispersion which must be adopted when we approximate by using classical mechanics. To this degree of approximation it is permissible to equate  $n^2\nu^2$  to  $\frac{2(E - F)mc^2}{h^2}$

and we obtain for the equation of a plane monochromatic wave of frequency  $\nu = \frac{mc^2 + E}{h}$  in the constant field defined by  $F(x, y, z)$  the non-relativistic form :

$$\nabla^2 \psi + \frac{8\pi^2 m(E - F)}{h^2} \psi = 0. \quad . \quad . \quad (27)$$

This is the now classical equation of Schrödinger.



#### 4. The Wave Equation in Variable Fields of Force

We have just found a suitable form for the equation of propagation for monochromatic waves in constant fields of force. This form, as we have already said, must be considered as a degeneration of a more general one, in which the frequency does not occur, and which is suitable not only in the case of a superposition of monochromatic waves but also in the case of fields of force which are variable in time.

The idea which must guide us in seeking this general equation is that to the approximation of geometrical optics, to be precise when  $h$  is supposed infinitely small, the equation of geometrical optics must be identified with Jacobi's equation, so that the phase  $\phi$  can be identified with Jacobi's function.

The general relativistic equation which satisfies this condition is the following :

$$\nabla^2\psi - \frac{1}{c^2} \frac{\partial^2\psi}{\partial t^2} + \frac{4\pi i}{hc^2} F \frac{\partial\psi}{\partial t} - \frac{4\pi^2}{h^2} \left( m^2 c^2 - \frac{F^2}{c^2} \right) \psi = 0, \quad (28)$$

in which  $F$  is a function of  $x, y, z$  and  $t$ .

For  $F = 0$  we obtain again equation (1). If  $F$  depends only upon  $x, y$  and  $z$ , and not upon  $t$ , we can take a monochromatic solution of the form :

$$\psi(x, y, z, t) = a(x, y, z) \cos 2\pi\{\nu t - \Phi_1(x, y, z)\} \quad (29)$$

and by making use of the complex form  $\psi = ae^{2\pi i(\nu t - \Phi_1)}$  we obtain :

$$\frac{\partial\psi}{\partial t} = 2\pi i\nu\psi, \quad \frac{\partial^2\psi}{\partial t^2} = -4\pi^2\nu^2\psi. \quad (30)$$

Equation (28) now takes the degenerate form :

$$\nabla^2\psi + \frac{4\pi^2\nu^2}{c^2} \psi - \frac{8\pi^2\nu}{hc^2} F\psi - \frac{4\pi^2}{h^2} \left( m^2 c^2 - \frac{F^2}{c^2} \right) \psi = 0, \quad (31)$$

which is identical with (11).

Let us consider the general case where  $F$  depends on the time or the case of the variable field. We shall show that if the function  $\psi$ , written in the complex form, satisfies equation (28) we can obtain Jacobi's equation in  $\phi$  if we suppose  $h$  to be infinitely small. By substitution of  $\psi = ae^{\frac{2\pi i}{h}\phi}$  in (28), and equating the real part to zero, we obtain :

$$\nabla^2 a - \frac{1}{c^2} \frac{\partial^2 a}{\partial t^2} - \frac{4\pi^2 a}{h^2} \left\{ \sum \left( \frac{\partial \phi}{\partial x} \right)^2 - \frac{1}{c^2} \left( \frac{\partial \phi}{\partial t} \right)^2 \right\} - \frac{8\pi^2 F}{h^2 c^2} a \frac{\partial \phi}{\partial t} - \frac{4\pi^2}{h^2} \left( m^2 c^2 - \frac{F^2}{c^2} \right) a = 0. \quad (32)$$

If  $h$  is supposed very small the terms containing  $\frac{1}{h^2}$  are of much greater importance than the others and, after removing a common factor, we obtain :

$$\frac{1}{c^2} \left( \frac{\partial \phi}{\partial t} - F \right)^2 - \sum \left( \frac{\partial \phi}{\partial x} \right)^2 = m^2 c^2, \quad (33)$$

and  $\phi$  thus satisfies the relativistic general equation of Jacobi (Chap. II, 32).

Equation (33) can be considered as being the equation of geometrical optics for the associated waves. As we have seen, if  $\phi(x, y, z, t, \alpha, \beta, \gamma)$  denotes a complete integral of this equation (33), the three relations :

$$\frac{\partial \phi}{\partial \alpha} = C_1, \quad \frac{\partial \phi}{\partial \beta} = C_2, \quad \frac{\partial \phi}{\partial \gamma} = C_3, \quad (34)$$

define the motion of states of phase agreement in a wave group and these three relations are nothing more than Jacobi's equations of motion. In this case also and in complete generality the motion of the particle, to the approximation of geometrical optics, can be regarded as that of a group of associated waves.

A very special characteristic of equation (28) is that it contains an imaginary coefficient and that, in order to satisfy it, the wave function must be taken in the complex form. In the equations of the classical wave theory the coefficients are real, and the real wave function,  $\psi = a \cos 2\pi\Phi$ , must satisfy the wave equation. The complex form of  $\psi$  is also a solution and the calculations are usually made by means of it, only, however, to return to the real part at the end. The use of the complex form in that case is merely a simple mathematical device. In the present theory this is by no means the case ; the real wave function does not satisfy equation (28), and the complex function itself is the solution.

Just as in the case of constant fields of force we passed from the relativistic equation (11) to the non-relativistic equation of Schrödinger (27), so we can in the general case pass from the relativistic equation (28) to a non-relativistic form.

We have to remind ourselves that in the dynamics of the theory of relativity the energy is given by :

$$W = \frac{mc^2}{\sqrt{1-\beta^2}} + F(x, y, z, t) = mc^2 + T + F = mc^2 + E, \quad (35)$$

$T$  being the kinetic and  $F$  the potential energy.  $E$  is the energy as defined in Newtonian dynamics, being equal to the relativistic energy diminished by the internal energy  $mc^2$ , and Newtonian dynamics is applicable when the ratio  $\frac{E}{mc^2}$  is small.

To carry this over into wave mechanics we write the wave function in the form :

$$\psi(x, y, z, t) = e^{\frac{2\pi i}{h} mc^2 t} \psi_r(x, y, z, t). \quad (36)$$

$\psi_r$  is thus the expression obtained on removing the term  $\frac{mc^2}{h}t$  from the phase of the complex wave, that is to say, by reducing the frequency from  $\frac{W}{h}$  to  $\frac{E}{h}$ .

We shall call  $\psi_r$  the reduced wave function, and  $\frac{E}{h}$  the reduced frequency. Substituting (36) in (28), we obtain :

$$\begin{aligned} \nabla^2 \psi_r - \frac{1}{c^2} \left( \frac{\partial^2 \psi_r}{\partial t^2} + \frac{4\pi i}{h} mc^2 \frac{\partial \psi_r}{\partial t} - \frac{4\pi^2}{h^2} m^2 c^4 \psi_r \right) \\ + \frac{4\pi i}{h c^2} F \left( \frac{\partial \psi_r}{\partial t} + \frac{2\pi i}{h} mc^2 \psi_r \right) - \frac{4\pi^2}{h^2} \left( m^2 c^2 - \frac{F^2}{c^2} \right) \psi_r = 0. \end{aligned} \quad (37)$$

The term containing  $F^2 \psi_r$  is negligible in comparison with that containing  $Fmc^2 \psi_r$ ; a similar remark applies to  $F \frac{\partial \psi_r}{\partial t}$  and  $mc^2 \frac{\partial \psi_r}{\partial t}$  and also to  $\frac{\partial^2 \psi_r}{\partial t^2}$  and  $mc^2 \frac{\partial \psi_r}{\partial t}$ , because all the derivatives of  $\psi_r$  with respect to the time are small compared with  $mc^2$ . Thus :

$$\nabla^2 \psi_r - \frac{8\pi^2}{h^2} m F \psi_r = \frac{4\pi i m}{h} \frac{\partial \psi_r}{\partial t}. \quad (38)$$

This is the non-relativistic equation <sup>1</sup> which the reduced wave function must satisfy.

<sup>1</sup> The non-relativistic wave equation is of the first order in  $t$ , while the relativity equation is of the second order in  $t$ . This is an important point of difference which Dirac has brought forward.

If the field does not depend on the time, we may write :

$$\psi_r = ae^{\frac{2\pi i}{h}(Et - \phi_1)} \quad . \quad . \quad . \quad (39)$$

where  $a$  and  $\phi_1$  are functions of  $x$ ,  $y$  and  $z$ , and we readily return once more to Schrödinger's equation (27).

Equation (38) is often written without the suffix  $r$ , but it must always be remembered that it is the reduced wave function of which the frequency is diminished by  $\frac{mc^2}{h}$  which is a solution of (38).

### 5. A Device for Finding Equation 38

We can find the non-relativistic wave-equation by making use of a device which is somewhat automatic and which has great importance in the comparison of Heisenberg's matrix theory with wave mechanics. We know that Jacobi's equation in Newtonian mechanics is :

$$H\left(q, t, -\frac{\partial S}{\partial q}\right) - \frac{\partial S}{\partial t} = 0, \quad . \quad . \quad (40)$$

(Chap. II, 9), where  $H\left(q, t, -\frac{\partial S}{\partial q}\right)$  denotes what the energy  $H$  becomes when expressed in terms of the co-ordinates  $q$ , of the time  $t$  and of the momenta  $p$  when the last are replaced by  $-\frac{\partial S}{\partial q}$ . If we take the first term of (40) and replace  $\frac{\partial S}{\partial q}$  by the symbol  $\frac{h}{2\pi i} \frac{\partial}{\partial q}$ , and  $\frac{\partial S}{\partial t}$  by  $\frac{h}{2\pi i} \frac{\partial}{\partial t}$ , we obtain an operator.

Now apply this operator to the reduced function  $\psi$  and equate to zero ; if the  $q$ 's are rectangular cartesian co-ordinates we obtain equation (38). We have, in fact, in this case :

$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2), \quad . \quad . \quad . \quad (41)$$

so that :

$$H(q, p, t) = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + F(x, y, z, t), \quad . \quad (42)$$

and Jacobi's equation is :

$$\frac{1}{2m}\left\{\left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2\right\} + F - \frac{\partial S}{\partial t} = 0. \quad . \quad (43)$$

The operator obtained by the method described is :

$$-\frac{\hbar^2}{8\pi^2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + F - \frac{\hbar}{2\pi i} \frac{\partial}{\partial t} \quad . \quad (44)$$

and we arrive at the wave equation :

$$\frac{1}{m}\nabla^2\psi - \frac{8\pi^2}{\hbar^2}F\psi = \frac{4\pi i}{\hbar} \frac{\partial\psi}{\partial t} \quad . \quad . \quad . \quad (45)$$

which is identical with (38). It may be easily verified that the same process applied to non-rectangular co-ordinates gives an incorrect wave equation.

## CHAPTER VI

### CLASSICAL MECHANICS AND WAVE MECHANICS

#### 1. The Meaning of Amplitude in Classical Mechanics

THE old systems of mechanics correspond, as we now know, to the case where the propagation of the  $\psi$ -waves follows the laws of geometrical optics. The phase function  $\phi$  can then be identified with Jacobi's function. But we have now to enquire what is the meaning to be attributed to the amplitude  $a$  if we wish provisionally to preserve the conception of particles localised in space.

We shall be content for the present with the study of the non-relativistic equations. Of course, these considerations will not be applicable to particles in very rapid motion, for example to light corpuscles, and when we consider the case of photons we shall have to resume our discussion.

Let us begin with the general non-relativistic equation

$$\nabla^2 \psi - \frac{8\pi^2 m}{h^2} F\psi = \frac{4\pi i m}{h} \frac{\partial \psi}{\partial t} \quad . \quad . \quad (1)$$

and substitute :

$$\psi = ae^{\frac{2\pi i}{h}\phi}, \quad . \quad . \quad . \quad . \quad (2)$$

$a$  and  $\phi$  being two real functions, the modulus and argument of the complex quantity  $\psi$ . We obtain by separating the real and imaginary parts :

$$-\nabla^2 a + \frac{4\pi^2}{h^2} a \sum \left( \frac{\partial \phi}{\partial x} \right)^2 + \frac{8\pi^2 m}{h^2} F a = \frac{8\pi^2 m}{h^2} a \frac{\partial \phi}{\partial t}, \quad . \quad (3)$$

$$\frac{4\pi i}{h} \sum \frac{\partial a}{\partial x} \frac{\partial \phi}{\partial x} + \frac{2\pi i}{h} \nabla a^2 \phi = \frac{4\pi i}{h} m \frac{\partial a}{\partial t}. \quad . \quad (4)$$

It follows from the discussions of Chapter IV (where  $\Phi = \frac{\phi}{h}$ ) that if geometrical optics is applicable, the term  $\nabla^2 a$  is negligible with respect to  $\frac{4\pi^2}{h^2} a \sum \left( \frac{\partial \phi}{\partial x} \right)^2$ . We can therefore write our equations (3) and (4) in the form :

$$\frac{1}{2m} \sum \left( \frac{\partial \phi}{\partial x} \right)^2 + F(x, y, z, t) = \frac{\partial \phi}{\partial t} \quad . \quad . \quad (5)$$

$$\text{and} \quad \sum \frac{\partial a}{\partial x} \frac{\partial \phi}{\partial x} + \frac{1}{2} a \nabla^2 \phi = m \frac{\partial a}{\partial t} \quad . \quad . \quad (6)$$

Equation (5) shows that  $\phi$  is identical with Jacobi's function, a result already known, and equation (6) will show us the meaning of  $a$ .

Let  $S(x, y, z, t, \alpha, \beta, \gamma)$  be a complete integral of Jacobi's equation where  $\alpha, \beta$  and  $\gamma$  are three constants. According to Jacobi's theory the equations of motion are :

$$\frac{\partial S}{\partial \alpha} = C_1, \quad \frac{\partial S}{\partial \beta} = C_2, \quad \frac{\partial S}{\partial \gamma} = C_3. \quad . \quad . \quad (7)$$

There is thus an infinite number of possible modes of motion of the particle which correspond to the same function of Jacobi, that is to say, correspond to the same value of the constants  $\alpha, \beta, \gamma$ , but with a different choice of the constants  $C_1, C_2, C_3$ . We shall say that these modes belong to the same class.

Instead of picturing a single particle describing a path, let us imagine an assembly of identical particles in motion in modes belonging to the same class. We know that the momenta  $p_x, p_y, p_z$  are deduced from  $S$  by the equations :

$$p_x = - \frac{\partial S}{\partial x}, \quad p_y = - \frac{\partial S}{\partial y}, \quad p_z = - \frac{\partial S}{\partial z}, \quad . \quad (8)$$

or vectorially :

$$\mathbf{p} = - \text{grad } S. \quad . \quad . \quad (9)$$

In Newtonian mechanics  $\mathbf{p} = m\mathbf{v}$ , hence :

$$\mathbf{v} = - \frac{1}{m} \text{grad } S. \quad . \quad . \quad (10)$$

Thus the motion of the cloud of particles is known completely if  $S$  is known. Since we may now identify  $\phi$  with  $S$ , equation (6) is equivalent to :

$$\frac{\partial a}{\partial t} + \sum v_x \frac{\partial a}{\partial x} + \frac{1}{2} a \operatorname{div} \mathbf{v} = 0. \quad (11)$$

By multiplication by  $2a$  we find at once :

$$\frac{\partial a^2}{\partial t} + \operatorname{div} (a^2 \mathbf{v}) = 0. \quad (12)$$

Moreover, the motion of the cloud of particles must satisfy the equation of continuity, which is the expression of the fact that the increase in number of particles in unit time in a region of space is equal to the difference between the number entering and leaving in that time.

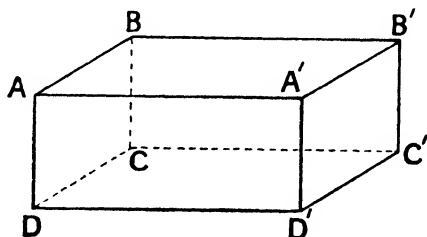


FIG. 2.

Let  $ABCD A'B'C'D'$  be a small parallelepiped with faces perpendicular to the axes of co-ordinates and with infinitesimal sides of lengths  $dx, dy, dz$ . Let  $\rho, v_x, v_y, v_z$  denote the density and velocity components of the cloud at the centre of the parallelepiped. The flux of particles in the interval  $dt$  across  $ABCD$  is  $\left\{ \rho v_x - \frac{1}{2} \frac{\partial}{\partial x} (\rho v_x) dx \right\} dt dy dz$ , and across  $A'B'C'D'$  in the same time the flux is  $\left\{ \rho v_x + \frac{1}{2} \frac{\partial}{\partial x} (\rho v_x) dx \right\} dt dy dz$ . Thus the excess of those entering over those leaving in this direction is  $-\frac{\partial}{\partial x} (\rho v_x) dt dx dy dz$ , and a similar calculation applied to the other pairs of faces shows that the total excess is

$$-\operatorname{div} (\rho \mathbf{v}) dt dx dy dz.$$



This must be equal to the increase during the time  $dt$  in the number  $\rho \, dx \, dy \, dz$  of particles present in the element of volume. This increase is  $\frac{\partial \rho}{\partial t} dt \, dx \, dy \, dz$ , so that we obtain the equation of continuity :

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0. \quad . \quad . \quad . \quad (13)$$

From a comparison of this equation with (12) we are led to write :

$$\rho = K a^2, \quad . \quad . \quad . \quad (14)$$

where  $K$  is a constant of proportionality which may be put equal to unity, since  $a$  may be multiplied by an arbitrary constant. We can thus say that the square of the amplitude of the  $\psi$ -wave or its intensity must be considered as measuring at each instant and at each point the density of the cloud of particles.

## 2. The Probability of Occurrence

The cloud of particles imagined in the preceding paragraph helps particularly in the visualisation of the assembly of possible modes of motion of the same class for a single particle. The density of this cloud may be considered as representing the probability that a particle, of which the mode of motion belongs to the class considered but of which the actual position is unknown, occupies a particular point at a particular time. Thus a restatement of the result obtained at the end of the last paragraph is that the intensity of the  $\psi$ -wave measures at each point at each instant the probability that the associated particle will occupy the point at the particular instant. This is the proposition which we described in the introduction as the principle of interference. We see that when the  $\psi$ -wave is propagated according to the laws of geometrical optics, the exactness of the principle is automatically guaranteed by the fact that under these conditions the laws of the old systems of mechanics are applicable to the motion of the particle.

The cloud of particles associated with one and the same wave appears therefore to be interpretable as a probability. We can consider this cloud as forming a fictitious fluid, the prob-

ability fluid, of which the density, equal to  $a^2$  by (14), gives at all points and times the probability of occurrence of the particle associated with the  $\psi$ -wave considered. The infinitely small portions of this fluid, the probability elements as we shall describe them, describe paths which coincide with possible paths of the particle of which the exact position is unknown. All this theory is very clear in the special case we are considering where geometrical optics is applicable for the propagation of the  $\psi$ -wave. We shall see that the difficulties begin when we leave the domain where geometrical optics applies.

We must underline one important point. The phase function is determined quite independently of the amplitude, and from this it follows by the equations of Jacobi's theory that the motion of the particle in its path is quite independent of the function  $a$ . This is necessary in order that we may agree with the old mechanics in considering the motion of the particle as being completely determined by the six initial conditions of position and velocity (i.e. the six constants of Jacobi's theory). Were the determination of  $\phi$  not independent of that of  $a$ , the form of  $\phi$  would depend on the values of that function at the different points of space at the initial instant, and this would mean that the motion of the particle would depend not only upon the initial conditions but also on the probability that the initial co-ordinates had this or that set of values. We shall see that it is this paradoxical circumstance which presents itself when we try to extend the ideas of the old mechanics to the domain proper of the new mechanics.

Let us consider closely the way in which the function  $a(x, y, z, t)$  must be determined when we assume that Jacobi's function  $S(x, y, z, t, \alpha, \beta, \gamma)$ , which is a complete integral of (5), is known. We must find a function satisfying (6) and such that at the initial instant  $t_0$ ,  $a(x, y, z, t_0)$  gives the probability of occurrence of the particle. If, for example, we have carried out an experiment at the instant  $t_0$  to determine the position of the particle, the result is always affected by a certain possible error, and must be expressed by saying that the probability that the particle was at the point  $(x, y, z)$  at time  $t_0$  is given by a function  $f(x, y, z)$ —the region of space where this function has a value appreciably different from zero being the smaller the more exact the experiment—we shall have therefore to

impose as an initial condition which the integral,  $a$ , of (6) must satisfy, the relation :

$$a^2(x, y, z, t_0) = f(x, y, z). \quad . \quad . \quad . \quad (15)$$

The meaning of  $f$  implies :

$$\int f dv = 1, \quad . \quad . \quad . \quad . \quad (16)$$

where the integral is taken over all space so that the function  $a$  always satisfies the condition :

$$\int a^2(x, y, z, t) dv = 1, \quad . \quad . \quad . \quad (17)$$

since the left-hand side of (17) measures the total probability that the particle occupies a point somewhere in space at time  $t$  and this total probability, being a certainty, is evidently unity.

### 3. Concrete Examples

We give two examples to make these points clear. Let us take first the case where there is no field of force. The plane monochromatic wave is then a solution of the wave-equation. Its amplitude is constant, which means that if we consider an infinite number of particles forming a homogeneous unlimited cloud, all moving with the same velocity, the density will undergo no change with the motion.

More instructive is the case of the motion of an unlimited cloud of particles with the same energy all moving in the direction of a uniform field of force acting upon them. We can describe all the phenomena by a single variable  $x$ .

If we resume the notation of Chapter II, § 6, we have :

$$F(x) = -kx \quad . \quad . \quad . \quad (18)$$

and the abscissa of each particle is given by :

$$x = x_0 + v_0 t + \frac{1}{2} \frac{k}{m} t^2, \quad . \quad . \quad . \quad (19)$$

$x_0$  being the abscissa and  $v_0$  the velocity of this particle at time  $t = 0$ . We have found that the complete integral of Jacobi's equation where  $W$  plays the part of an arbitrary constant is :

$$S(x, t, W) = Wt - \frac{1}{3mk} \{2m(kx + W)\}^{\frac{3}{2}}. \quad . \quad (20)$$

Moreover, equation (6), in which we may replace  $\phi$  by  $S$ , gives us :

$$\frac{\partial a}{\partial x} \frac{\partial S}{\partial x} + \frac{1}{2} a \frac{\partial^2 S}{\partial x^2} = m \frac{\partial a}{\partial t}. \quad (21)$$

As we are determining the motion of an indefinite cloud of particles, we may suppose the motion permanent in such a way that  $a$  is independent of the time. Then (21) will become simpler and we have :

$$\frac{\partial a}{\partial x} \frac{\partial S}{\partial x} + \frac{1}{2} a \frac{\partial^2 S}{\partial x^2} = 0. \quad (22)$$

Now, by (20) :

$$\frac{\partial S}{\partial x} = -\sqrt{2m(kx + W)}, \quad \frac{\partial^2 S}{\partial x^2} = \frac{-mk}{\sqrt{2m(kx + W)}}, \quad (23)$$

thus the amplitude  $a$  must satisfy the equation :

$$\frac{1}{a} \frac{da}{dx} = -\frac{k}{4(kx + W)} \quad (24)$$

of which the integral is

$$a = C(kx + W)^{-\frac{1}{4}} \quad (25)$$

where  $C$  is a constant.

By (14) the density of the cloud is therefore :

$$\rho = a^2 = \frac{C}{\sqrt{kx + W}} = \rho_0 \frac{\sqrt{kx_0 + W}}{\sqrt{kx + W}}, \quad (26)$$

where  $\rho_0$  is the value of  $\rho$  for a certain value  $x_0$  of  $x$ .

The density of the cloud thus diminishes in the direction of the field. Since we are considering a case where wave mechanics and the old mechanics are identical, we ought to be able to find (26) by means of the classical equations of motion. We proceed to show that this is possible.

Let us fix our attention upon a certain abscissa  $x_0$  and upon the particles to be found in the plane  $x_0$  at the instant  $t = 0$ . These particles begin with a velocity  $v_0$ , and at time  $t$  they will have reached the plane with abscissa  $x = x_0 + v_0 t + \frac{1}{2} \frac{k}{m} t^2$ , by (19). The particles lying in the plane  $(x_0 - \delta x_0)$  had a velocity

$v_0 - \delta v_0$  at  $t = 0$ , and at time  $t$  they will have reached the plane with abscissa :

$$x' = (x_0 - \delta x_0) + (v_0 - \delta v_0)t + \frac{1}{2} \frac{k}{m} t^2. \quad (27)$$

Thus the particles which at zero time occupied a cylinder of unit cross-section bounded by the planes  $x_0$  and  $x_0 - \delta x_0$  will occupy at  $t$  a cylinder of the same cross-section bounded by the planes  $x$  and  $x'$ . If  $N$  is the number of corpuscles within these limits, the density at  $x_0$  is

$$\rho_0 = \frac{N}{\delta x_0} \quad . \quad . \quad . \quad (28)$$

and at  $x$  :

$$\rho = \frac{N}{x - x'} = \frac{N}{\delta x_0 + v_0 t} = \frac{N}{\delta x_0} \cdot \frac{1}{1 + \frac{\delta v_0 t}{\delta x_0}} = \frac{\rho_0}{1 + \frac{\delta v_0 t}{\delta x_0}}. \quad (29)$$

But since by hypothesis all the particles of the cloud have the same energy  $W$ , the velocity and abscissa of each particle are related by the equation :

$$\frac{1}{2} m v^2 - kx = W \quad . \quad . \quad . \quad (30)$$

or 
$$v = \sqrt{\frac{2(W + kx)}{m}}. \quad . \quad . \quad . \quad (31)$$

Since  $\delta v_0$  is the variation which the velocity undergoes for a change of  $\delta x_0$  in the abscissa, we have by (31) :

$$\delta v_0 = \frac{k \delta x_0}{\sqrt{2m(W + kx_0)}} \quad . \quad . \quad . \quad (32)$$

and (29) becomes :

$$\rho = \frac{\rho_0}{1 + \frac{kt}{\sqrt{2m(kx_0 + W)}}} = \rho_0 \frac{\sqrt{kx_0 + W}}{\sqrt{kx_0 + W} + \frac{kt}{\sqrt{2m}}}. \quad (33)$$

We have also :

$$v = v_0 + \frac{k}{m} t \quad . \quad . \quad . \quad (34)$$

and by (31) :

$$\sqrt{kx + W} = \sqrt{kx_0 + W} + \frac{kt}{\sqrt{2m}}, \quad . \quad . \quad (35)$$

so that we obtain finally for  $\rho$  the expression :

$$\rho = \rho_0 \frac{\sqrt{kx_0 + W}}{\sqrt{kx + W}}, \quad . \quad . \quad . \quad (36)$$

and this is the formula (26) obtained from the amplitude of the associated wave.

#### 4. Summary of the Chapter

We have thus established a parallelism between the old mechanics and the propagation of the  $\psi$ -waves when this proceeds according to the laws of geometrical optics.

Jacobi's function then becomes identical with the phase function of the  $\psi$ -waves, and if we preserve the classical concept of particles describing well-defined paths with definite velocities, we may imagine a cloud of particles describing all the paths which correspond to one and the same function of Jacobi, in which case the density of the cloud can always be measured by the intensity of the associated wave. We may also imagine a probability fluid the elements of which describe the paths which correspond to a given form of Jacobi's function, and we may say that the density of this fluid measures at each point of space and time the probability of occurrence of a single particle. Our information about this particle is only that it describes one of the paths, but we do not know which.

All these conceptions are in this case clear and quite in harmony with classical ideas, but is it possible to extend them when the conditions of geometrical optics do not prevail? We shall see that we must at all cost hold to the view that the intensity of the  $\psi$ -wave measures the probability of occurrence of the particle, even if our effort makes us sacrifice the traditional idea which gives to the particles a position, a velocity and a well-defined path.

## CHAPTER VII

### THE PRINCIPLE OF INTERFERENCE AND THE DIFFRACTION OF ELECTRONS BY CRYSTALS

#### 1. The Principle of Interference

THE essential principle which is used in the theory of light to anticipate the results of an experiment in interference or diffraction is that the square of the amplitude, or the intensity, is a measure of the quantity of luminous energy which is present on the average at each point of space. Further, the optical experiments on interference have always given the same result however feeble the intensity of the light used. Thus if we admit the existence of particles of luminous energy, or photons, it is necessary to suppose that for each photon the probability of occurrence is proportional at each point to the intensity of the luminous wave associated with them, this is what we describe as the principle of interference. As we have said in the introduction, it is quite natural in wave mechanics to try to take over this principle from the case of light to that of material particles, that is, to admit that the intensity of the  $\psi$ -wave always measures the probability of occurrence of the particle at a particular point of space and time, even though the principles of geometrical optics may not be applicable to the propagation of this wave. Let  $P(x, y, z, t)dv$  denote the probability that the particle lies at time  $t$  within the element of volume  $dv$ , and let  $(x, y, z)$  denote the co-ordinates of the centre of this element. By writing :

$$\psi(x, y, z, t) = a(x, y, z, t)e^{\frac{2\pi i}{h}\phi(x, y, z, t)}, \quad . \quad . \quad (1)$$

we have :

$$P = Ka^2 = K\psi\bar{\psi}, \quad . \quad . \quad . \quad (2)$$

$\bar{\psi}$  denoting the complex conjugate of  $\psi$ . By a convenient choice of the arbitrary constant factor of  $a$  we may make  $K = 1$ .

The relation (2) is the expression of the principle of interference.

All experiments which have been carried out with particles under conditions where the propagation of the associated waves proceeds according to the laws of geometrical optics verify of necessity the principle of interference, as follows from the preceding chapter. To obtain experimental proof of the general value of the principle it is therefore necessary to turn to phenomena where the associated wave propagation proceeds no longer according to these laws. This is exactly what takes place in experiments on diffraction of electrons by crystals. These experiments may be considered as supplying at one and the same time proof of the necessity of introducing associated waves and proof of the exactness of the principle of interference in its application to material particles.

## 2. The Diffraction of Electrons

Davisson and Germer have the honour of being the first to obtain diffraction of electrons by crystals. They directed a beam of electrons, all having the same velocity, normally on the face of a nickel crystal, this face of incidence being one of the faces of the regular octahedron of the cubical system of nickel. The electrons first used by Davisson and Germer were very slow ones of 50 to 200 volts; later these American physicists extended their researches to electrons of several hundred volts. The results obtained showed very clearly that there was a concentration of electrons scattered in the directions in which the associated wave is expected to present a maximum as a result of the agreement in phase between the waves diffracted by the different crystal centres. The phenomenon is thus exactly comparable with that of Laue for X-rays. The numerical values have, moreover, indicated clearly that a wave-length of magnitude

$$\lambda = \frac{h}{mv} \quad . \quad . \quad . \quad . \quad (3)$$



must be attributed to the associated wave, as was indicated by the general theory of Chapter III. Nevertheless, certain differences were found between the results of the experiment and the deductions from the theory of Bragg and Laue obtained by applying (3). It seems possible to explain these differences by taking into account the possibility that within the crystal the index of refraction for the electron waves differs appreciably from that in empty space.

Experiments of the same kind have been very brilliantly repeated by Professor G. P. Thomson in a different way. He made use of a method exactly analogous to that of Debye and Sherrer for X-rays by using electrons of great velocities, obtained by subjecting them to potentials of some thousands of volts. Under these circumstances the complications due to the refractive index of the crystals disappear. We have, in fact, found that in a field in which the potential function is  $F(x, y, z)$  the refractive index of the associated wave is

$$n = \sqrt{\frac{2(E - F)}{mc^2}}. \quad . \quad . \quad . \quad (4)$$

Outside the field  $F = 0$  and the index is :

$$n_0 = \sqrt{\frac{2E}{mc^2}}. \quad . \quad . \quad . \quad (5)$$

The refractive index of the crystal with respect to empty space for the associated waves of an electron with energy  $E$  is thus :

$$\frac{n}{n_0} = \sqrt{1 - \frac{F}{E}}, \quad . \quad . \quad . \quad (6)$$

$F$  being the potential energy of the electron at the point  $(x, y, z)$ , due to its interaction with the centres of the crystalline medium. Since  $F$  does not depend upon  $E$  it is evident that  $\frac{n}{n_0}$  approaches the value unity as  $E$  increases indefinitely.

In the experiments of Davisson and Germer the refractive index  $\frac{n}{n_0}$  could have differed from unity by nearly  $\frac{1}{10}$  ; for the electrons in Thomson's experiment, which were 50 to 100 times faster than those in the former, the difference between  $\frac{n}{n_0}$  and

unity was negligible. We shall see in detail further on that the results were quite in agreement with the theory of Bragg and Laue and with formula (3).

Other very remarkable experiments on the diffraction of electrons have been made in Germany by Rupp, who caused slow electrons to pass through metal films. Here again the theory was verified, but with a slight systematic deviation which was attributed to the refractive index. Quite recently, Rupp, making use of the method so successfully applied by Thibaud for X-rays, was able to diffract a beam of electrons at grazing incidence on an ordinary optical grating. The formula (3) was again verified with great exactness, and the wave-length of the associated electron wave has thus been measured directly by a ruled grating.

In the present work it is impossible to examine in detail all the experimental results, which are already numerous. We shall limit ourselves to the study of Thomson's experiments which are free from the difficulty with regard to the refractive index. For the other experiments the reader is referred to the original memoirs. The essential point for us is that experiment has provided a wonderful confirmation both of the existence of associated electron waves and of the formula for the wave-length in terms of the velocity. It has also shown the validity of the principle of interference, even in its application to material particles.

### 3. Preliminaries to the Study of G. P. Thomson's Experiments

The method of G. P. Thomson is to send an approximately homogeneous beam of electrons across a very thin metal film. We regard such a film nowadays as made up of very small crystals joined together. In order to see to what phenomenon the scattering of waves by these crystals must give rise we must first recall some of the notions of crystallography.

Since the work of Bravais we regard all crystals as formed of material centres arranged according to regular laws in the form of a lattice. The simplest type of lattice is that in which any displacement of the form  $n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$  causes one crystalline centre to be carried over to another,  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  being three vectors not all in the same plane and  $n_1$ ,  $n_2$ ,  $n_3$  being

any three integers. The centres or nuclei thus form the corners of an infinite number of parallelepipeds situated side by side. If we consider two nuclei, A and B, of a simple lattice, the displacement which makes one pass into the others is thus of the form  $n(h\mathbf{a} + j\mathbf{b} + k\mathbf{c})$ , where  $n$  is an integer, while  $h, j, k$  are three integers with no common factor. The straight line AB thus carries an infinite number of centres which may be derived from one another by means of the displacement  $h\mathbf{a} + j\mathbf{b} + k\mathbf{c}$ . It follows that any plane containing three nuclei not in a straight line contains an infinite number of nuclei at the corners of adjacent parallelograms; such a plane is called reticular. If a reticular plane is subject to a displacement  $n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$  we obtain another parallel reticular plane, and thus the reticular planes form a system of parallel planes. In order to describe a family of reticular planes we will take three co-ordinate axes passing through a nucleus of the lattice and parallel respectively to the three vectors  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$ . We will then consider that plane of the family closest to the origin which cuts the three axes in three nuclei situated on the positive sides. This plane cuts the  $x$ -axis at the point  $m_1a$ , the  $y$ -axis at  $m_2b$  and the  $z$ -axis at  $m_3c$ . The indices of the family of reticular planes considered are the smallest whole numbers  $(h_1, h_2, h_3)$  which are proportional to the reciprocals of  $(m_1, m_2, m_3)$ .

The plane which serves to define the numbers  $(m_1, m_2, m_3)$  is represented by the equation :

$$\frac{x}{m_1a} + \frac{y}{m_2b} + \frac{z}{m_3c} = 1. \quad . \quad . \quad (7)$$

Let  $k$  denote the lowest common multiple of  $m_1, m_2$  and  $m_3$ , then :

$$h_1 = \frac{k}{m_1}, \quad h_2 = \frac{k}{m_2}, \quad h_3 = \frac{k}{m_3}, \quad . \quad . \quad (8)$$

and equation (7) may be written :

$$h_1\frac{x}{a} + h_2\frac{y}{b} + h_3\frac{z}{c} = k. \quad . \quad . \quad (9)$$

All the reticular planes of the same family have therefore an equation of the form :

$$h_1\frac{x}{a} + h_2\frac{y}{b} + h_3\frac{z}{c} = \text{constant}. \quad . \quad . \quad (10)$$

Now it is easy to see that a plane of the family considered passes through every nucleus of the lattice. Suppose that  $P$  is a plane passing through a nucleus  $A$ , and let  $B$  be another nucleus not lying in  $P$ . We pass from  $A$  to  $B$  by a displacement  $n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$ , and this displacement transforms  $P$  into a parallel plane  $P'$  passing through  $B$ . Every nucleus situated in  $P$  is transformed to one situated in  $P'$ . The plane  $P'$ , which contains an infinite number of nuclei, is a reticular plane of the same family as  $P$ , and it passes through the nucleus  $B$  which is chosen arbitrarily.

With the notation just used we proceed to calculate the distance between parallel planes  $P$  and  $P'$ , but we shall make the restriction that the vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  are mutually perpendicular, since this is the only case to which we shall have to apply our formulæ. Let  $A$  be the origin of co-ordinates so that the plane  $P$  has for its equation :

$$h_1\frac{x}{a} + h_2\frac{y}{b} + h_3\frac{z}{c} = 0 \quad . \quad . \quad . \quad (11)$$

where  $(h_1, h_2, h_3)$  are the indices of the family of planes of which  $P$  is a member. The co-ordinates of  $B$  are  $(n_1a, n_2b, n_3c)$ , and since the co-ordinates are rectangular the distance from  $B$  to the plane  $P$  is given by the formula of analytical geometry :

$$d = \frac{h_1n_1 + h_2n_2 + h_3n_3}{\sqrt{\left(\frac{h_1}{a}\right)^2 + \left(\frac{h_2}{b}\right)^2 + \left(\frac{h_3}{c}\right)^2}} \quad . \quad . \quad . \quad (12)$$

$B$  may be any nucleus whatever, that is to say, we may choose for  $(n_1, n_2, n_3)$  any whole numbers, positive or negative, and the numerator of (12) may consequently have any integral value. Thus we conclude that the reticular planes of the family  $(h_1, h_2, h_3)$  are equidistant from one another with a separation

$$d_{h_1h_2h_3} = \frac{1}{\sqrt{\left(\frac{h_1}{a}\right)^2 + \left(\frac{h_2}{b}\right)^2 + \left(\frac{h_3}{c}\right)^2}} \quad . \quad . \quad . \quad (13)$$

In the case of a cubic lattice  $a = b = c$  and :

$$d_{h_1h_2h_3} = \frac{a}{\sqrt{h_1^2 + h_2^2 + h_3^2}} \quad . \quad . \quad . \quad (14)$$

The simple cubic lattice is formed by nuclei situated at the corners of an infinite number of cubes in juxtaposition. It is defined by three vectors ( $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ ) mutually perpendicular and of the same length  $a$ . The most important families of reticular planes are :

(100) cube faces.

(111) faces of octahedra.

(110) faces of dodecahedra.

The corresponding equidistances are :

$$d_{100} = a, \quad d_{111} = \frac{a}{\sqrt{3}}, \quad d_{110} = \frac{a}{\sqrt{2}}.$$

But it often happens that actual cubic lattices have a more complicated structure. It may happen, for example, that each elementary cube carries not only nuclei at the corners, but also a nucleus at its centre and we then have a lattice of centred cubes.

It is just as if we had two simple cubic lattices displaced from one another by  $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ . The most general displacement which then makes one nucleus pass into another is  $(n_1 + \frac{\epsilon_1}{2})\mathbf{a} + (n_2 + \frac{\epsilon_2}{2})\mathbf{b} + (n_3 + \frac{\epsilon_3}{2})\mathbf{c}$ , where  $(n_1, n_2, n_3)$  are integers and  $(\epsilon_1, \epsilon_2, \epsilon_3)$  are equal to 0 or 1. If we repeat the argument above in this case we find that the separation of the planes of a family ( $h_1, h_2, h_3$ ) is :

$$\left. \begin{aligned} d_{h_1 h_2 h_3} &= \frac{a}{\sqrt{h_1^2 + h_2^2 + h_3^2}} \text{ if } (h_1 + h_2 + h_3) \text{ is even} \\ \text{and } d_{h_1 h_2 h_3} &= \frac{1}{2} \frac{a}{\sqrt{h_1^2 + h_2^2 + h_3^2}} \text{ if } (h_1 + h_2 + h_3) \text{ is odd.} \end{aligned} \right\} \quad (15)$$

Finally, and this is the case in Thomson's experiments, we may have a cubic lattice in which each elementary cube carries a nucleus at the centre of each of its six faces ; this is a face-centred lattice. The most general displacement which carries one nucleus into another is now

$$(n_1 + \frac{\epsilon_1}{2})\mathbf{a} + (n_2 + \frac{\epsilon_2}{2})\mathbf{b} + (n_3 + \frac{\epsilon_3}{2})\mathbf{c},$$

where the  $n$ 's have the same significance as before, but the  $\epsilon$ 's are either all zero or two have the values unity and the third

is zero. The distance from a nucleus B to a reticular plane passing through A is :

$$d = \frac{\left(n_1 + \frac{\epsilon_1}{2}\right)h_1 + \left(n_2 + \frac{\epsilon_2}{2}\right)h_2 + \left(n_3 + \frac{\epsilon_3}{2}\right)h_3}{\sqrt{h_1^2 + h_2^2 + h_3^2}}. \quad (16)$$

If the  $h$ 's are all odd or all even, we have :

$$d_{h_1 h_2 h_3} = \frac{a}{\sqrt{h_1^2 + h_2^2 + h_3^2}}, \quad (17)$$

while if odd and even values of the  $h$ 's occur, we have :

$$d_{h_1 h_2 h_3} = \frac{1}{2} \cdot \frac{a}{\sqrt{h_1^2 + h_2^2 + h_3^2}} = \frac{a}{\sqrt{(2h_1)^2 + (2h_2)^2 + (2h_3)^2}}. \quad (18)$$

Thus we may say that (17) applies in the latter case provided the indices are doubled.

#### 4. Experiments of G. P. Thomson

Let us return to G. P. Thomson's experiments and suppose that a homogeneous beam of cathode rays in its passage through a thin metal film encounters in one of the small crystals of which the film is composed a plane with indices  $(h_1, h_2, h_3)$  at an angle of incidence  $\theta$ , where  $\theta$  denotes the complement of the angle of incidence usually considered in optics. The wave associated with the incident electrons will undergo a strong scattering in the direction of regular reflection if there is agreement in phase amongst the elementary waves scattered by the nuclei of the different reticular planes of indices  $(h_1, h_2, h_3)$ .

In the first place, the waves scattered by two centres A and B lying in the same reticular plane are always in phase in the direction of regular reflection, since the optical paths A'B and AB' are equal, both having the value  $AB \cos \theta$  (Fig. 3).

If, further, the waves scattered by two centres A and C, situated as in the figure, are in phase, the waves scattered by all the nuclei of the crystal will be in phase and we shall have in the direction of regular reflection a large maximum of intensity. The condition for this is that the optical paths of the ray scattered by A and of that scattered by C differ by an integral multiple of the wave-length. This gives :

$$DC + CD' = n\lambda \quad (n = \text{an integer}),$$

i.e.

$$2d_{h_1h_2h_3} \sin \theta = n\lambda. \quad (19)$$

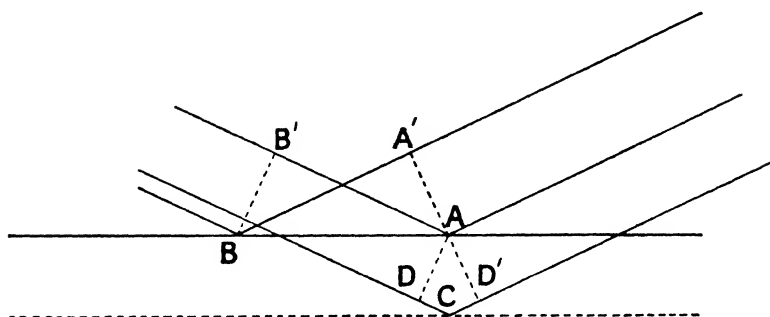
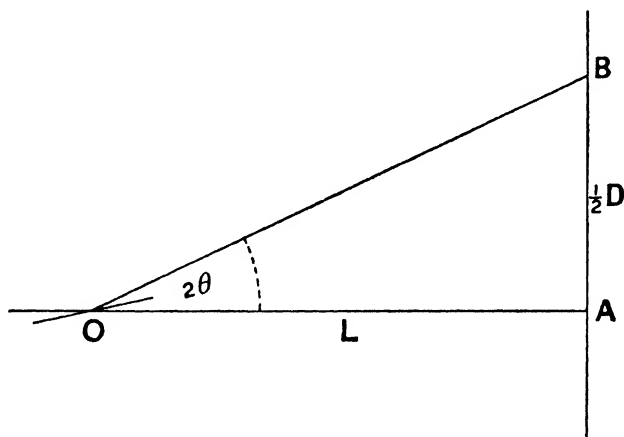


FIG. 3.

This is the well-known relation of Bragg for X-rays. His demonstration assumes that the difference between the idea of refraction for the crystal and for empty space may be neglected,



$$OA = L; AB = \frac{1}{2}D.$$

FIG. 4.

and we have seen that this is a legitimate assumption for the case of Thomson's experiments.

Let  $L$  be the distance from the metal film to the photographic plate on which the electrons are received. We expect

to obtain for each reflection on a small crystal a small spot at a distance  $\frac{D}{2}$  from the direction of the cathode beam, where

$\frac{D}{2} = L \tan 2\theta$ , if the principle of interference holds for the electrons, that is to say, if the square of the amplitude of the wave measures the probability of occurrence of electrons at each point.

The wave-length  $\lambda$  of the wave associated with the incident electrons is the magnitude which controls this phenomenon. From the general formulæ :

$$\lambda = \frac{h}{p} = \frac{h}{mv} \sqrt{1 - \beta^2}. \quad (20)$$

The velocity of the electrons is determined by the potential difference  $P$  applied to put them in motion. We have :

$$\frac{mc^2}{\sqrt{1 - \beta^2}} - mc^2 = eP, \quad (21)$$

whence

$$\frac{1}{1 - \beta^2} - 1 = \frac{\beta^2}{1 - \beta^2} = \frac{2eP}{mc^2} + \frac{e^2 P^2}{m^2 c^4} \quad (22)$$

and

$$\frac{\sqrt{1 - \beta^2}}{\beta c} = \frac{1}{\sqrt{\frac{2eP}{m} + \frac{e^2 P^2}{m^2 c^2}}}, \quad (23)$$

whence finally :

$$\lambda = \frac{h}{\sqrt{2meP \left(1 + \frac{eP}{2mc^2}\right)}}. \quad (24)$$

The term  $\frac{eP}{2mc^2}$  is always small, so that it is sufficient to write :

$$\lambda = \frac{h}{\sqrt{2meP}} \left(1 - \frac{eP}{4mc^2}\right), \quad (25)$$

and in this formula the value of  $e$  is  $-4.77 \times 10^{-10}$  e.s.u.

If  $P$  be expressed in volts (25) must be replaced by :

$$\lambda = h \sqrt{\frac{150}{meP}} \left(1 - \frac{eP}{1200mc^2}\right). \quad (26)$$



In Thomson's experiments the correction term was never greater than 3 per cent., so that we may write as an approximate formula :

$$\lambda = h\sqrt{\frac{150}{meP}}, \quad . \quad . \quad . \quad (27)$$

which can be obtained directly from the non-relativistic relations

$$\lambda = \frac{h}{mv} \quad \text{and} \quad \frac{1}{2}mv^2 = eP.$$

By applying the foregoing relations we find for 25,000 volt electrons the value  $0.75 \times 10^{-9}$  cms. for the wave-length, which shows that the electronic waves correspond to very hard X-rays. As the ordinary crystal lattices have plane separations of the order of  $10^{-8}$  cms., the angles  $\theta$  will be very small, and it will be sufficient to replace  $\sin \theta$  and  $\tan 2\theta$  in the formulæ by  $\theta$  and  $2\theta$  respectively. We have, therefore, approximately :

$$2d\theta = n\lambda \quad \text{and} \quad \frac{D}{2} = L \cdot 2\theta,$$

whence

$$D = \frac{2n\lambda L}{d_{h_1h_2h_3}}. \quad . \quad . \quad . \quad (28)$$

If the microcrystals of the film are oriented by chance, we shall obtain on the photographic plate not a spot but an infinite number of spots describing a continuous ring, of diameter  $D$ , about the line of incidence of the beam. If the metal film contains microcrystals presenting any degree of specialised orientation, we shall have more complicated appearances, certain rings being absent others interrupted. This has been observed. It must be noted that the films should be very thin in order that the electron beam should not be too much absorbed nor subject to multiple scattering.

The first experiments carried out by Thomson as a test were made on aluminium and gold. One of the first things to be verified is that for a given ring, i.e. one produced by a particular family of reticular planes, the ratio  $\frac{D}{\lambda}$  is constant. In other words, if the tension  $P$  is progressively increased, the

ring system will contract and if the contraction of a ring be followed, the relation

$$\frac{D}{\lambda} = \text{constant},$$

or

$$D\sqrt{P}\left(1 + \frac{eP}{1200 mc^2}\right) = \text{constant} \quad . \quad (29)$$

must be verified.

The following are tables of values given by Thomson :—

*Aluminium*

P (volts).	D (cms.).	$D\sqrt{P}\left(1 + \frac{eP}{1200 mc^2}\right)$ .
64,000	1.47	384
57,600	1.62	398
45,000	1.78	388
34,500	2.00	378

*Gold*

58,000	1.50	371
55,000	1.58	381
44,000	1.75	376
33,700	2.00	374

*Platinum*

45,000	1.85	402
40,000	1.96	400
34,500	2.23	421
25,500	2.46	398

*Aluminium (with another value of L)*

34,500	1.64	310
27,500	1.84	310
26,200	1.86	305
21,800	2.09	312

*Platinum (with another value of L)*

29,000	1.84	319
24,000	1.98	311

The variation of wave-length with the potential P and consequently with the velocity of the electrons is thus well verified.

For a particular potential, D and D' corresponding to the reflections on reticular planes with indices ( $h_1, h_2, h_3$ ) and ( $h_1', h_2', h_3'$ ) are in the ratio :

$$\frac{D'}{D} = \frac{d_{h_1 h_2 h_3}}{d_{h_1' h_2' h_3'}}. \quad . \quad . \quad . \quad (30)$$

Since the metals used crystallise in the face-centred cubic system, we have :

$$d_{h_1 h_2 h_3} = \frac{a}{\sqrt{h_1^2 + h_2^2 + h_3^2}}, \quad . \quad . \quad (31)$$

$a$  being the edge of the cube and the indices being doubled if they are not all odd or all even. Thus with this convention :

$$\frac{D'}{D} = \frac{\sqrt{h_1'^2 + h_2'^2 + h_3'^2}}{\sqrt{h_1'^2 + h_2'^2 + h_3'^2}}. \quad . \quad . \quad (32)$$

In a series of experiments on aluminium, Thomson obtained rings with diameters proportional to :

$$\begin{array}{cccccc} \sqrt{4}, & \sqrt{8\cdot00}, & \sqrt{10\cdot9}, & \sqrt{16\cdot5}, & \sqrt{27}, \\ \sqrt{4}, & \sqrt{7\cdot65}, & \sqrt{10\cdot6}, & \sqrt{14\cdot8}, & \\ \sqrt{4}, & \sqrt{8\cdot05}, & \sqrt{11\cdot05}, & \sqrt{15\cdot8}, & \sqrt{28}, \\ \sqrt{4}, & \sqrt{7\cdot93}, & \sqrt{11\cdot4}, & \sqrt{16}, & \\ \sqrt{4}, & \sqrt{7\cdot95}, & \sqrt{10\cdot8}, & \sqrt{15\cdot8}, & \sqrt{26\cdot6}, \\ \sqrt{4}, & \sqrt{8\cdot00}, & \sqrt{10\cdot9}, & \sqrt{15\cdot4}, & \sqrt{27\cdot4}. \end{array}$$

This series is a good approximation to the series :

$$\sqrt{4}, \quad \sqrt{8}, \quad \sqrt{11}, \quad \sqrt{16}, \quad \sqrt{27},$$

which corresponds to the reticular planes :

$$200, \quad 220, \quad 311, \quad 400, \quad 511.$$

In the same way the following series has been found for platinum :

$$\begin{array}{cccccccc} \sqrt{3}, & \sqrt{4\cdot00}, & \sqrt{7\cdot95}, & \sqrt{11\cdot1}, & \sqrt{16\cdot2}, & \sqrt{18\cdot8}, & \sqrt{23\cdot2}, & \sqrt{26\cdot8}, \\ \sqrt{3}, & \sqrt{4\cdot05}, & \sqrt{8\cdot05}, & \sqrt{11\cdot4}, & \sqrt{15\cdot2}, & \sqrt{18\cdot4}, & \sqrt{22\cdot5}, & \sqrt{26\cdot3}, \\ \sqrt{3}, & \sqrt{3\cdot98}, & \sqrt{7\cdot95}, & \sqrt{10\cdot8}, & \sqrt{15\cdot2}, & \sqrt{18\cdot3}, & \sqrt{23\cdot8}, & \sqrt{26\cdot4}, \end{array}$$

and these correspond to the series :

$$\sqrt{3}, \quad \sqrt{4}, \quad \sqrt{8}, \quad \sqrt{11}, \quad \sqrt{16}, \quad \sqrt{19}, \quad \sqrt{24}, \quad \sqrt{27},$$

associated with the reticular planes :

$$111, \quad 200, \quad 220, \quad 311, \quad 400, \quad 331, \quad 422, \quad 333.$$

We have similarly two series for gold :

$$\begin{array}{cccccc} \sqrt{3}, & \sqrt{4\cdot2}, & \sqrt{7\cdot9}, & \sqrt{11\cdot5}, & \sqrt{19\cdot9}, \\ \sqrt{3}, & \sqrt{4\cdot08}, & \sqrt{8}, & \sqrt{11\cdot1}, & \sqrt{19\cdot9}, \end{array}$$

which are very close to the series :

$$\sqrt{3}, \sqrt{4}, \sqrt{8}, \sqrt{11}, \sqrt{20},$$

corresponding to the planes :

$$111, 200, 220, 311, 420.$$

Having in this way found the indices of the reflecting planes, we can calculate the edges of the cubes and compare the results with the values found in X-ray experiments. The results are :

	Al.	Au.	Pt.
For cathode rays, $a =$	$4.035\text{\AA}$ ,	$4.20\text{\AA}$ ,	$3.89\text{\AA}$ .
For X-rays, $a =$	$4.063\text{\AA}$ ,	$4.06\text{\AA}$ ,	$3.91\text{\AA}$ .

Thomson also verified, in a very interesting way, that the production of impressions on the photographic plate was by electrons scattered by the film and not by secondary X-rays. This was done by establishing a magnetic field between the film and the plate and observing the displacement of the ring pattern as a whole by the action of the field. He was, in this way, able to verify that the velocity of the scattered electrons was equal to that of those incident.

The first of Thomson's experiments were carried out with a celluloid film, and gave definite results but rather qualitative in character. One of his pupils, Mr. Reid, has since resumed these experiments and found a good agreement with theory by assuming the existence of two plane separations of  $3.67\text{\AA}$  and  $4.35\text{\AA}$ , while the distances measured by Müller for the fatty acids are  $3.67\text{\AA}$  and  $4.08\text{\AA}$ . Finally, another collaborator of Thomson's, Mr. Ironside, has also obtained a confirmation of the theory for films of copper, silver and tin, metals which crystallise also in face-centred cubes. The following are examples of the values of the sides of the elementary cubes which he has obtained compared with those obtained with X-rays :

	Ag.	Cu.	Sn.
For cathode rays, $a =$	$4.11\text{\AA}$ ,	$3.66\text{\AA}$ ,	$2.86\text{\AA}$ .
For X-rays, $a =$	$4.08\text{\AA}$ ,	$3.60\text{\AA}$ ,	$2.91\text{\AA}$ .

## CHAPTER VIII

### THE PRINCIPLE OF INTERFERENCE AND THE SCATTERING OF CHARGED PARTICLES BY A FIXED CENTRE

#### 1. The Scattering of Charged Particles According to Classical Mechanics

WE pass on to another example of the value of the principle of interference in its application to material particles ; we shall in fact show that the principle of interference applied to electrified particles gives Rutherford's law for the scattering of these particles in their passage through matter, a law which has been verified by experiment (Rutherford and Chadwick). We will begin with the classical method by which Rutherford established the law, then by means of a calculation by Wentzel we will show that we arrive at the same result by using the ideas of wave mechanics and the principle of interference.

Let  $e$  and  $m$  denote the charge and mass of the incident particles,  $e_1$  the charge of the scattering centre, supposed fixed, close to which the incident particles pass in traversing the matter. We shall suppose, in accordance with the conditions of the experiment, that in the beginning the charged particles all move with the same velocity  $\mathbf{v}$  in a certain direction. We will take the position of the fixed centre as origin and the direction of the initial motion as the axis of  $x$  (Fig. 5).

Once out of the region where the action of the centre is appreciable, each particle will again move in a straight line with a uniform velocity  $\mathbf{v}$  but in a direction which makes a certain angle with the original direction of motion. The principle of conservation of moment of momentum about  $O$  gives :

$$m v b = - m r^2 \frac{d\theta}{dt}, \quad . \quad . \quad . \quad (1)$$

$(r, \theta)$  being the polar co-ordinates of the particle at time  $t$  and  $b$  the initial distance from the polar axis.

Again, taking account of Coulomb's law, the equation of motion along  $Oy$  perpendicular to  $Ox$  is :

$$m \frac{dv_y}{dt} = \frac{ee_1}{r^2} \sin \theta = -\frac{ee_1}{bv} \sin \theta \cdot \frac{d\theta}{dt} \quad (2)$$

Integrating :

$$mv \sin \alpha = \frac{ee_1}{vb} (1 + \cos \alpha), \quad (3)$$

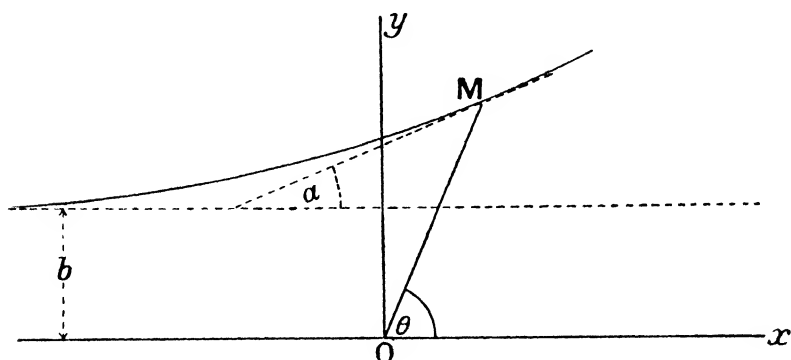


FIG. 5.

where the limits are for  $\theta$ ,  $\pi$  to  $\alpha$ , and for  $v_y$ , 0 to  $v \sin \alpha$ .

From (3) we find :

$$b = \frac{ee_1}{mv^2 \sin \alpha} (1 + \cos \alpha) = \frac{ee_1}{mv^2} \cot^2 \frac{\alpha}{2} \quad (4)$$

Now the probability that the distance between the initial trajectory and the  $x$ -axis should lie between  $b$  and  $b + db$  is clearly  $2\pi b db$  multiplied by a constant. It is also equal to the probability  $P(\alpha) d\alpha$  that the final angle made with  $x$ -axis should lie within the range  $\alpha$  to  $(\alpha + d\alpha)$ , which corresponds according to (4) to the range  $b$  to  $b + db$ . Taking account of the fact that  $\alpha$  and  $b$  vary in opposite senses, we have :

$$P(\alpha) d\alpha = -A 2\pi b db = -B \frac{db^2}{d\alpha} d\alpha = -B \frac{e^2 e_1^2}{m^2 v^4} \frac{d}{d\alpha} \left( \cot^2 \frac{\alpha}{2} \right) d\alpha, \quad (5)$$

where  $A$  is a constant and  $B = \pi A$ .

The number of particles undergoing a deviation included between  $\alpha_1$  and  $\alpha_2$  is proportional to  $\left(\cot^2 \frac{\alpha_1}{2} - \cot^2 \frac{\alpha_2}{2}\right)$ , which is Rutherford's law. There is, however, a difficulty, for if we integrate (5) from 0 to  $\alpha_0$  we see that the number of particles undergoing a deviation less than  $\alpha_0$  is infinitely great. This may appear to be an objection to the result of the calculation, but it is not so, for we have in fact implicitly supposed the incident beam of particles unlimited laterally, and if this is so there would be an infinite number of particles passing far enough from the centre to undergo no appreciable deviation. But in practice the beams of particles are always limited laterally, so that the calculation no longer applies to large values of  $b$ , that is to say, to small values of  $\alpha$ , and it is precisely for these small values of  $\alpha$  that  $\int P(\alpha) d\alpha$  diverges.

## 2. The Calculation by means of Wave Mechanics

Let us now take the point of view of the new mechanics. We must associate with the incident particles the wave :

$$\psi_0(x, t) = a_0 e^{\frac{2\pi i}{h}(Wt - mvx)}, \quad . \quad . \quad . \quad (6)$$

where  $a_0$  is a constant and where  $W$  has the value :

$$W = mc^2 + \frac{1}{2}mv^2 = mc^2 + E, \quad . \quad . \quad . \quad (7)$$

the second term being very small relatively to the first if we restrict ourselves to the Newtonian approximation as in the preceding paragraph. The wave-length has the value :

$$\lambda = \frac{h}{mv}, \quad . \quad . \quad . \quad (8)$$

and under the usual experimental conditions it is always very small and of the order of that of X-rays.

In the neighbourhood of the scattering centre, O, a field of force with a potential function  $F(r)$  exists, and the wave-equation is :

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - F) \psi = 0. \quad . \quad . \quad (9)$$

When the  $\psi$ -waves enter this region we have a condition similar to that which occurs when a light wave enters a non-homogeneous refracting medium ; a scattered wave is superposed upon the incident wave  $\psi_0$ .

We suppose that the scattering does not appreciably enfeeble the incident wave, whence :

$$\psi = \psi_0 + \psi_1, \quad \psi_1 \ll \psi_0 \quad . \quad . \quad . \quad (10)$$

Since  $\psi_0$  satisfies the equation :

$$\nabla^2 \psi_0 + \frac{8\pi^2 m}{h^2} E \psi_0 = 0 \quad . \quad . \quad . \quad (11)$$

the scattered wave is an approximate solution of the equation :

$$\nabla^2 \psi_1 + \frac{8\pi^2 m}{h^2} E \psi_1 = \frac{8\pi^2 m}{h^2} F \psi_0, \quad . \quad . \quad . \quad (12)$$

a result which follows from (9) and (10). Now, since the frequency  $\frac{W}{h}$  is approximately equal to  $\frac{mc^2}{h}$  for the incident as for the scattered wave, we have :

$$\frac{\partial^2 \psi_1}{\partial t^2} = - \frac{4\pi^2 m^2 c^4}{h^2} \psi_1 \quad \text{or} \quad \frac{8\pi^2 m}{h^2} \psi_1 = - \frac{2}{mc^4} \frac{\partial^2 \psi_1}{\partial t^2}, \quad (13)$$

and substituting (13) in (12),

$$\nabla^2 \psi_1 - \frac{2E}{mc^4} \frac{\partial^2 \psi_1}{\partial t^2} = \frac{8\pi^2 m}{h^2} F \psi_0. \quad . \quad . \quad (14)$$

Since  $2E = mv^2$ , we have :

$$\nabla^2 \psi_1 - \frac{1}{V^2} \frac{\partial^2 \psi_1}{\partial t^2} = \frac{8\pi^2 m}{h^2} F \psi_0, \quad . \quad . \quad (15)$$

where

$$V = \frac{c^2}{v}. \quad . \quad . \quad . \quad (16)$$

$\psi_0(x, t)$  and  $F(r)$  being given in this problem, the equation (15) is of the form :

$$\nabla^2 \psi_1 - \frac{1}{V^2} \frac{\partial^2 \psi_1}{\partial t^2} = \sigma(x, y, z, t), \quad . \quad . \quad (17)$$

where

$$\sigma(x, y, z, t) = \frac{8\pi^2 m}{h^2} F(r) \psi_0(x, t). \quad . \quad . \quad (18)$$



The solution of (17) is given by Kirchhoff's well-known formula of retarded potentials :

$$\psi_1 = -\frac{1}{4\pi} \iiint \left[ \frac{\sigma}{\rho} \right]_{t-\frac{\rho}{V}} d\tau, \quad (19)$$

$d\tau$  being an element of volume surrounding a point M of the region of integration, and  $\rho$  denoting the distance PM, where P is the point for which  $\psi_1$  is calculated at a time  $t$ . The suffix  $\left(t - \frac{\rho}{V}\right)$  denotes that  $\frac{\sigma}{\rho}$  has its value, not at the instant  $t$ , but at the instant  $\left(t - \frac{\rho}{V}\right)$ . In this case we must write :

$$[F\psi_0]_{t-\frac{r}{V}} = F(r)a_0 e^{2\pi i\left(\frac{Wt}{h} - \frac{x+\rho}{\lambda}\right)}, \quad (20)$$

and therefore from (18) and (19) :

$$\psi_1 = -\frac{2\pi m}{h^2} a_0 e^{\frac{2\pi i Wt}{h}} \iiint \frac{F}{\rho} e^{-\frac{2\pi i}{\lambda}(x+\rho)} d\tau. \quad (21)$$

A difficulty arises here, for it would be natural to write :

$$F(r) = \frac{ee_1}{r} \quad (22)$$

since the action of the scattering centre on the incident particles follows Coulomb's law. If, however, we use this relation, the integral of (21) will be divergent, as we shall see from our calculation. To avoid this difficulty, Wentzel has written :

$$F(r) = \frac{ee_1}{r} e^{-kr}, \quad (23)$$

$k$  having the property that  $k\lambda \ll 1$ . In a region surrounding the centre O and of dimensions large compared with the wavelength, the expression (23) is approximately identical with that of Coulomb. But in regions far removed from O the exponential factor is appreciable and the rapid decrease in  $F$  with increase in  $r$  prevents infinite scattering. We believe that it is possible to interpret Wentzel's device in the following way. By representing the incident wave as plane and monochromatic we thereby assume the incident beam to be actually unlimited, and this cannot correspond to anything occurring in practice.

The incident beam is necessarily limited laterally, and it would have to be represented by a train of waves of finite dimensions. If we wish to simplify the calculation by representing the incident beam by a monochromatic wave, we must of necessity correct the error thereby introduced, and this is done by introducing Wentzel's exponential factor to annul the influence of the distant portions of the monochromatic wave, these portions having in fact no real existence.

Let us accept Wentzel's hypothesis and calculate the scattered wave at a point P very distant from O (Fig. 6).

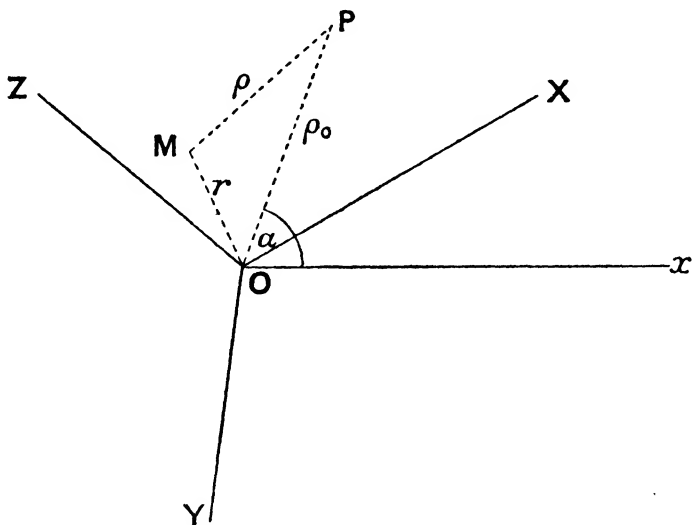


FIG. 6.

On account of the factor  $e^{-kr}$  the integration (21) concerns only the immediate neighbourhood of O ; we may thus replace  $\rho$  by  $OP = \rho_0$  in the slowly varying factor  $\frac{1}{\rho}$ , and in the exponential factor write :

$$\rho = \rho_0 - r \cos \widehat{POM}. \quad . \quad . \quad . \quad (24)$$

The equation (21) now becomes :

$$\psi_1 = - \frac{2\pi m}{\hbar^2} \cdot e e_1 \frac{a_0}{\rho_0} e^{2\pi i \left( \frac{W}{h} t - \frac{\rho_0}{\lambda} \right)} \iiint \frac{e^{-kr + \frac{2\pi i}{\lambda} (r \cos \widehat{MOP} - x)}}{\bar{r}} d\tau. \quad (25)$$

Choose a system of rectangular co-ordinates (X, Y, Z) such that the plane XOZ coincides with the plane xOP and let OX and OZ be the internal and external bisectors respectively of the angle  $\hat{xOP} = \alpha$ . Let OY be perpendicular to the plane xOP. The polar co-ordinates of M are  $(r, \theta, \phi)$ , with OZ as the polar axis. In the system (X, Y, Z) the direction cosines of O $\hat{x}$ , OM, OP are given by the following table :

	OX.	OY.	OZ.
O $\hat{x}$ . . .	$\cos \frac{\alpha}{2}$	0	$-\sin \frac{\alpha}{2}$
OM . . .	$\sin \theta \cos \phi$	$\sin \theta \sin \phi$	$\cos \theta$
OP . . .	$\cos \frac{\alpha}{2}$	0	$\sin \frac{\alpha}{2}$

Thus :

$$\left. \begin{aligned} \cos \hat{POM} &= \sin \theta \cos \phi \cos \frac{\alpha}{2} + \cos \theta \sin \frac{\alpha}{2} \\ x = r \cos \hat{MOx} &= r \left( \sin \theta \cos \phi \cos \frac{\alpha}{2} - \cos \theta \sin \frac{\alpha}{2} \right) \\ r \cos \hat{MOP} - x &= 2r \cos \theta \sin \frac{\alpha}{2} \end{aligned} \right\} \quad (26)$$

The integral in (25) becomes, therefore,

$$\int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \int_0^\infty e^{-kr + \frac{4\pi i}{\lambda} r \cos \theta \sin \frac{\alpha}{2}} r dr. \quad (27)$$

The integration with respect to  $\phi$  gives  $2\pi$ . On integrating by parts with respect to  $r$ , noting that the real part of the exponent is negative, we find for the integral in  $r$  the value :

$$\frac{1}{\left(-k + \frac{4\pi i}{\lambda} \sin \frac{\alpha}{2} \cos \theta\right)^2}, \quad (28)$$

or approximately :

$$-\frac{1}{\frac{16\pi^2}{\lambda^2} \sin^2 \frac{\alpha}{2} \cos^2 \theta}, \quad (29)$$

on account of the order of magnitude of  $k$ .

We have also :

$$\int_0^\pi \frac{\sin \theta d\theta}{\cos^2 \theta} = \left( \frac{1}{\cos \theta} \right)_0^\pi = -2, \quad (30)$$

so that finally the value of (27) is :

$$\frac{\lambda^2}{4\pi \sin^2 \frac{\alpha}{2}}. \quad (31)$$

Substituting (31) in (25) we have :

$$\psi_1 = - \frac{\lambda^2 m e e_1}{2\hbar^2} \frac{a_0}{\rho_0 \sin^2 \frac{\alpha}{2}} e^{2\pi i \left( \frac{W}{h} t - \frac{\rho_0}{\lambda} \right)}, \quad (32)$$

and since  $\frac{m\lambda^2}{\hbar^2} = \frac{1}{mv^2}$ , the square of the amplitude at P of the scattered wave has the value :

$$a_1^2 = \frac{e^2 e_1^2}{4m^2 v^4} \frac{a_0^2}{\rho_0^2 \sin^4 \frac{\alpha}{2}}. \quad (33)$$

Let us consider the sphere with centre O and radius  $\rho_0$ . The number of scattered particles traversing the spherical zone corresponding to the angular interval  $\alpha$  to  $(\alpha + d\alpha)$  per unit time must be :

$$\frac{e^2 e_1^2}{4m^2 v^4} \frac{a_0^2}{\rho_0^2 \sin^4 \frac{\alpha}{2}} \cdot v \cdot 2\pi \rho_0^2 \sin \alpha d\alpha = \frac{\pi e^2 e_1^2}{2m^2 v^4} \cdot \frac{a_0^2}{\sin^4 \frac{\alpha}{2}} v \sin \alpha d\alpha \quad (34)$$

since  $a_1^2$  measures the density of the cloud of scattered particles. Moreover, the number of particles crossing a wave front,  $x = \text{constant}$ , per unit time situated far away on the left of the centre O is clearly proportional to  $a_0^2 v$ . The probability of a deviation between  $\alpha$  and  $(\alpha + d\alpha)$  is therefore :

$$\begin{aligned} P(\alpha) d\alpha &= A \frac{e^2 e_1^2}{m^2 v^4} \cdot \frac{1}{\sin^4 \frac{\alpha}{2}} \cdot 2 \sin \frac{\alpha}{2} \cos \frac{\alpha}{2} d\alpha \\ &= -A \frac{e^2 e_1^2}{m^2 v^4} \cdot \frac{d}{d\alpha} \left( \cot^2 \frac{\alpha}{2} \right) d\alpha, \end{aligned} \quad (35)$$

where A is a constant.

We thus determine again Rutherford's formula, and as it has been verified by experiment we have here another example where the principle of interference applied to material particles gives a result in agreement with observation.

Our method of procedure has introduced approximations, but Gordon has shown that Rutherford's formula may be obtained rigorously without approximation in the determination of the wave-scattering

## CHAPTER IX

### THE MOTION OF THE PROBABILITY WAVE IN THE NEW MECHANICS

#### 1. The Probability Cloud

WE saw in Chapter VI that in the limiting case, where the approximations of geometrical optics were applicable to the propagation of the associated wave, that is to say, in the limiting case of the old mechanics, it was possible to imagine a probability fluid moving in space so that its density was a measure at each point of space and time of the probability of occurrence of the particle.

We shall see that this is also valid in complete generality in the new mechanics if we accept the principle of interference which is confirmed by the diffraction of electrons by crystals.

We shall develop these ideas by the application of the non-relativistic equations.

We begin therefore with the wave equation :

$$\nabla^2 \psi - \frac{8\pi^2 m}{h^2} F \psi = \frac{4\pi i m}{h} \frac{\partial \psi}{\partial t}, \quad . \quad . \quad (1)$$

and we substitute :

$$\psi(x, y, z, t) = a(x, y, z, t) e^{\frac{2\pi i}{h} \phi}, \quad . \quad . \quad (2)$$

where  $\phi$  also is a function of  $x, y, z, t$ , and  $a$  and  $\phi$  are real functions.

In this way we obtain, as we have already seen (Chap. VI (3) and (4)) two equations which may be written thus :

$$\frac{1}{2m} \sum \left( \frac{\partial \phi}{\partial x} \right)^2 + F(x, y, z, t) - \frac{h^2}{8\pi^2 m} \frac{\nabla^2 a}{a} = \frac{\partial \phi}{\partial t}, \quad . \quad (3)$$

$$\sum \frac{\partial a}{\partial x} \frac{\partial \phi}{\partial x} + \frac{1}{2} a \nabla^2 \phi = m \frac{\partial a}{\partial t}. \quad . \quad . \quad (4)$$

In the present case  $a$  and  $\phi$  can only be determined simultaneously, a circumstance in which it differs from that occurring in the approximation of geometrical optics. All the equations being of the first order in the time, the function  $\psi(x, y, z, t)$  will be determined if we know its form  $\psi(x, y, z, 0)$  at the origin of time. Let us suppose that we have in this way determined the function  $\psi(x, y, z, t)$  and consequently the functions  $a$  and  $\phi$ . Let us imagine a probability fluid of which the molecules or, perhaps preferably, the elements possess the mass  $m$  of the particle studied. Equation (4) shows, as in Chapter VI, that by attributing to the elements the velocity defined by :

$$\mathbf{v} = -\frac{1}{m} \text{grad } \phi, \quad . \quad . \quad . \quad (5)$$

the density  $\rho$  of the probability cloud will always remain proportional to  $a^2(x, y, z, t)$  if it was equal to  $a^2(x, y, z, 0)$  initially. By (5) we can write (4) :

$$\frac{\partial a^2}{\partial t} + \text{div}(a^2 \mathbf{v}) = 0 \quad . \quad . \quad . \quad (6)$$

and this expresses the condition of continuity if we write  $\rho = K a^2$ . The constant  $K$  will be determined by the condition that  $\iiint K a^2 dv$  extended throughout the probability cloud is equal to unity, and since  $a$  by its definition may have a constant factor, we may include  $K$  in  $a^2$  and say that the cloud density is equal to the square of the amplitude of the  $\psi$ -wave.

We can consider (3) as Jacobi's equation for the motion of the probability elements, their potential energy being  $F + F_1$  where :

$$F_1(x, y, z, t) = -\frac{\hbar^2}{8\pi^2 m} \frac{\nabla^2 a}{a}. \quad . \quad . \quad (7)$$

This potential energy depends on the cloud density, and we can say that in order to obtain the motion of the probability elements, it is necessary to add the supplementary potential (7) to the ordinary potential  $F$ . Since  $F_1$  depends upon  $\hbar$  and is negligible when  $\hbar$  is regarded as an infinitely small quantity, we may describe it as the quantum potential.

## 2. Equations of Motion of the Probability Elements

If we regard equation (3) as the Jacobi equation for the probability elements we are naturally led to introduce a Lagrangian function depending upon their co-ordinates, velocities and the time. This function will be :

$$L(x, y, z, v_x, v_y, v_z, t) = \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2) - F - F_1. \quad (8)$$

The quantities

$$\frac{\partial L}{\partial v_x} = mv_x, \quad \frac{\partial L}{\partial v_y} = mv_y, \quad \frac{\partial L}{\partial v_z} = mv_z. \quad (9)$$

may be called the components of the momentum of the probability elements. The quantity

$$W = \sum \frac{\partial L}{\partial \dot{q}_n} \dot{q}_n - L = \frac{1}{2}mv^2 + F + F_1 \quad (10)$$

may be described as the energy of the elements.

By (5) we shall have :

$$p_x = mv_x = -\frac{\partial \phi}{\partial x}, \text{ etc. } \quad (11)$$

The elements describe a path in space according to a certain law and their motion is described by equations like those of Lagrange. We have :

$$\frac{dp_x}{dt} = \frac{\partial p_x}{\partial x} v_x + \frac{\partial p_x}{\partial y} v_y + \frac{\partial p_x}{\partial z} v_z + \frac{\partial p_x}{\partial t} = \frac{1}{m} \sum p_x \frac{\partial p_x}{\partial x} + \frac{\partial p_x}{\partial t}, \quad (12)$$

or by (11) :

$$\left. \begin{aligned} \frac{dp_x}{dt} &= \frac{1}{m} \sum \frac{\partial \phi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial x \partial t} \\ &= \frac{\partial}{\partial x} \left\{ \frac{1}{2m} \sum \left( \frac{\partial \phi}{\partial x} \right)^2 - \frac{\partial \phi}{\partial t} \right\} \end{aligned} \right\} \quad (13)$$

Since  $\phi$  is a solution of (3),

$$\frac{dp_x}{dt} = -\frac{\partial F}{\partial x} - \frac{\partial F_1}{\partial x} = \frac{\partial L}{\partial x}, \quad (14)$$

and similarly :

$$\frac{dp_y}{dt} = -\frac{\partial F}{\partial y} - \frac{\partial F_1}{\partial y} = \frac{\partial L}{\partial y}, \quad (15)$$

$$\frac{dp_z}{dt} = -\frac{\partial F}{\partial z} - \frac{\partial F_1}{\partial z} = \frac{\partial L}{\partial z}. \quad (16)$$



The terms  $\left(\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y}, \frac{\partial F}{\partial z}\right)$  are the force components in the classical sense, while  $\left(\frac{\partial F_1}{\partial x}, \frac{\partial F_1}{\partial y}, \frac{\partial F_1}{\partial z}\right)$  are derived from the quantum potential  $F_1$  in a way similar to the derivation of the former from the classical potential  $F$ , and may be described as the components of the quantum force. This force depends on the density of the probability fluid, and is characteristic of the new mechanics. When it can be neglected we return to the old dynamics and the motions of the probability elements are the various classical motions possible for the particle.

When it is not permissible to neglect the quantum force, the motion of the elements is very different from that of particles in the old dynamics. In particular we shall no longer find the general theorems of conservation of energy and momentum associated with them.

For example, if we consider the case of zero field ( $F = 0$ ), it does not follow that  $p_x, p_y, p_z$  are constants on account of the occurrence of the quantum force in equations (14)-(16).

Whenever the  $\psi$ -wave is not plane and monochromatic, for example if there is a superposition of plane waves with interference, the amplitude is not constant, and although there is no field in the old sense of the word, there will be, nevertheless, a variation of the components of momenta as defined by (11). There is thus no longer conservation of momentum. Further, by (9), (10), and (14)-(16) there is no longer conservation of energy, for :

$$\begin{aligned} \frac{dW}{dt} &= \sum \left( p_x \frac{d^2 x}{dt^2} + \frac{dp_x}{dt} \cdot \frac{dx}{dt} \right) - \sum \frac{\partial L}{\partial x} \frac{dx}{dt} - \sum \frac{\partial L}{\partial v_x} \frac{dv_x}{dt} - \frac{\partial L}{\partial t} \\ &= - \frac{\partial L}{\partial t} = \frac{\partial F}{\partial t} + \frac{\partial F_1}{\partial t}. \end{aligned} \quad (17)$$

It will not be sufficient to have  $\frac{\partial F}{\partial t} = 0$ , as occurs in a constant field, in order that there may be conservation of energy ; it will be necessary also for the amplitude of the  $\psi$ -wave to be independent of the time and this is not the case when  $\psi$  is a superposition of plane monochromatic waves. The probability motion does not proceed in general, even in the absence of an

external field, with conservation of energy and momentum, and the cause of this is the existence of the quantum force.

### 3. The Theorem of Ehrenfest

It is possible to eliminate the quantum force by means of an integration extended to the assembly of probability elements, and in so doing to arrive at an important theorem due to Ehrenfest. Multiply equations (14) to (16) by  $a^2 dx dy dz$  and integrate throughout space under the assumption that we are concerned with a limited wave train, the amplitude of which is consequently zero at infinity. We obtain :

$$\begin{aligned} \iiint a^2 \frac{dp_x}{dt} dx dy dz &= - \iiint a^2 \frac{\partial F}{\partial x} dx dy dz - \iiint a^2 \frac{\partial F_1}{\partial x} dx dy dz \\ &= - \iiint a^2 \frac{\partial F}{\partial x} dx dy dz + \iiint \frac{h^2}{8\pi^2 m} a^2 \frac{\partial}{\partial x} \left( \frac{\nabla^2 a}{a} \right) \\ &\quad dx dy dz, \quad (18) \end{aligned}$$

and two similar equations in  $y$  and  $z$ , where the integration is extended over all values of the variables.

We shall show that the integral

$$\iiint a^2 \frac{\partial}{\partial x} \left( \frac{\nabla^2 a}{a} \right) dx dy dz$$

and the two similar to it vanish. To show this we must remember one of the forms of Green's theorem that if  $U$  and  $V$  are two continuous uniform functions of  $(x, y, z)$  within a domain  $D$  bounded by a closed surface  $S$ , we have :

$$\iiint_D (U \nabla^2 V - V \nabla^2 U) dv = \iint_S \left( U \frac{\partial V}{\partial n} - V \frac{\partial U}{\partial n} \right) dS. \quad (19)$$

where  $n$  denotes the variable along the normal to  $S$  reckoned positive towards the exterior. Let us write :

$$U = a, \quad V = \frac{\partial a}{\partial x}. \quad . \quad . \quad . \quad (20)$$

These functions are by hypothesis both zero at infinity, and if we take, as the domain  $D$ , the interior of a sphere whose radius

tends to infinity, the right-hand side vanishes. We obtain, therefore :

$$\iiint a \nabla^2 \left( \frac{\partial a}{\partial x} \right) dv = \iiint \frac{\partial a}{\partial x} \nabla^2 a dv, \quad (21)$$

where the integrals are taken over the infinite domain D.

But the integral

$$\iiint a^2 \frac{\partial}{\partial x} \left( \frac{\nabla^2 a}{a} \right) dv$$

may be written :

$$\iiint \left( a \frac{\partial}{\partial x} (\nabla^2 a) - \frac{\partial a}{\partial x} \nabla^2 a \right) dv,$$

and this vanishes by (21). Equation (14) thus leads to :

$$\iiint a^2 \frac{dp_x}{dt} dv = m \iiint a^2 \frac{d^2 x}{dt^2} dv = - \iiint a^2 \frac{\partial F}{\partial x} dv = \iiint a^2 f_x dv. \quad (22)$$

We can take the cloud density equal to  $a^2$  provided that we choose the arbitrary constant factor of  $a$  so that :  $\iiint a^2 dv = 1$ . The integrals (22) are thus the average values in the probability cloud of the quantities  $\frac{dp_x}{dt}$ ,  $\frac{d^2 x}{dt^2}$ ,  $-\frac{\partial F}{\partial x}$  and  $f_x$ .

We obtain from (22) and the two similar equations which may be derived from (15) and (16) the relations :

$$\overline{\frac{dp_x}{dt}} = m \overline{\gamma_x} = \overline{f_x} \text{ and two similar ones in } y \text{ and } z, \quad (23)$$

where the bars denote average quantities.

This is Ehrenfest's theorem, of which we shall have later an interesting application.<sup>1</sup>

<sup>1</sup> If we write  $\bar{x} = \iiint a^2 x dv$ , we can easily show that  $\frac{d^2 \bar{x}}{dt^2} = \overline{\frac{d^2 x}{dt^2}}$ , with similar equations in  $y$  and  $z$ ; (23) may be written :

$$m \frac{d^2 \bar{x}}{dt^2} = \overline{f_x}, \text{ etc.}$$

We can state Ehrenfest's theorem by saying that the centre of gravity of the probability cloud moves like a particle of mass  $m$  in classical mechanics under the force with components  $(\overline{f_x}, \overline{f_y}, \overline{f_z})$ .

If the classical force is zero we have :

$$\overline{\frac{dp_x}{dt}} = 0, \quad \overline{\frac{dp_y}{dt}} = 0, \quad \overline{\frac{dp_z}{dt}} = 0, \quad . \quad . \quad . \quad (24)$$

and we find in this case a theorem analogous to that of conservation of momentum of the classical theory. This is due to the fact that we have eliminated the quantum force by means of an integration throughout the whole of the cloud.

In the same way, we can obtain a theorem analogous to that of conservation of energy. From (17) we have :

$$\frac{dW}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F_1}{\partial t}.$$

Multiply by  $a^2 dv$  and integrate throughout space assuming  $a$  zero at infinity, then :

$$\iiint a^2 \frac{dW}{dt} dv = \iiint a^2 \frac{\partial F}{\partial t} dv + \iiint a^2 \frac{\partial F_1}{\partial t} dv. \quad . \quad (25)$$

From (7) :

$$\iiint a^2 \frac{\partial F_1}{\partial t} dv = - \frac{h^2}{8\pi^2 m} \iiint a^2 \frac{\partial}{\partial t} \left( \frac{\nabla^2 a}{a} \right) dv. \quad . \quad (26)$$

The integral (26) is zero, for by substituting in Green's formula (19) :

$$U = a, \quad V = \frac{\partial a}{\partial t}, \quad . \quad . \quad . \quad (27)$$

we obtain :

$$\iiint a \nabla^2 \left( \frac{\partial a}{\partial t} \right) dv = \iiint a \frac{\partial}{\partial t} (\nabla^2 a) dv = \iiint \frac{\partial a}{\partial t} \nabla^2 a dv. \quad (28)$$

Thus the integral (26) vanishes, since :

$$\iiint a^2 \frac{\partial}{\partial t} \left( \frac{\nabla^2 a}{a} \right) dv = \iiint \left\{ a \frac{\partial}{\partial t} (\nabla^2 a) - \nabla^2 a \frac{\partial a}{\partial t} \right\} dv. \quad . \quad (29)$$

The equation (25) is thus reduced to :

$$\iiint a^2 \frac{dW}{dt} dv = \iiint a^2 \frac{\partial F}{\partial t} dv, \quad . \quad . \quad (30)$$

and if the field is constant  $\left( \frac{\partial F}{\partial t} = 0 \right)$ , we have :

$$\iiint a^2 \frac{dW}{dt} dv = \frac{dW}{dt} = 0. \quad . \quad . \quad (31)$$

The formula (31) is the statement of a theorem analogous to that of conservation of energy.

#### 4. Calculation of the Functions $\phi$ and $a$

If the wave function is known in the form :

$$\psi = ae^{\frac{2\pi i \phi}{h}}, \quad . \quad . \quad . \quad . \quad (32)$$

where  $a$  and  $\phi$  are real, the motion of the probability cloud and its density are determined by the formulæ of the first two paragraphs. But it often happens that  $\psi$  is known in the form :

$$\psi = \sum_k a_k e^{\frac{2\pi i}{h} \phi_k}, \quad (33)$$

which in the case of constant fields corresponds to spectral decomposition into monochromatic waves. It is thus useful to know how to calculate  $a$  and  $\phi$  when the wave function is given in the form (33). Let us denote the complex conjugate quantity corresponding to  $\psi$  by  $\psi^*$ . We have :

$$\psi^* = ae^{-\frac{2\pi i}{h}\phi} = \sum_k a_k e^{-\frac{2\pi i}{h}\phi_k}. \quad (34)$$

**Multiplying  $\psi$  by  $\psi^*$  :**

$$\begin{aligned} \alpha^2 &= \psi\psi^* = \sum_{kl} a_k a_l e^{\frac{2\pi i}{h}(\phi_k - \phi_l)} \\ &= \sum_k a_k^2 + \sum_{l < k} a_k a_l \cos \frac{2\pi}{h}(\phi_k - \phi_l). \end{aligned} \quad (35)$$

This formula determines the resultant intensity which, according to the principle of interference, gives the probability of occurrence.

If we divide  $\psi$  by  $\psi^*$ , and take the logarithm of the quotient, we obtain :

$$\phi = \frac{\hbar}{4\pi i} \log \frac{\psi}{\psi^*} = \frac{\hbar}{4\pi i} \log \frac{\sum_k a_k e^{\frac{2\pi i}{\hbar} \phi_k}}{\sum_k a_k e^{-\frac{2\pi i}{\hbar} \phi_k}}. \quad (36)$$

Let  $q$  denote any one of the four variables  $x, y, z, t$ , then :

$$\frac{\partial \phi}{\partial q} = \frac{\hbar}{4\pi i} \frac{\psi^*}{\psi} \cdot \frac{\psi^* \frac{\partial \psi}{\partial q} - \psi \frac{\partial \psi^*}{\partial q}}{\psi^{*2}} = \frac{\hbar}{4\pi i} \frac{\psi^* \frac{\partial \psi}{\partial q} - \psi \frac{\partial \psi^*}{\partial q}}{a^2}. \quad (37)$$

This formula gives us at the same time the components of  $\text{grad } \phi$  and the derivative  $\frac{\partial \phi}{\partial t}$  which represent respectively the components of momentum and the energy of the probability elements.

### 5. The Pilot-Wave Theory

We have seen that in the domain of application of geometrical optics we can consider the probability cloud as equivalent to a cloud of particles in a state of motion in the given field corresponding to one and the same complete integral of Jacobi's equation. We can also consider one particle only and say that the probability cloud is obtained by imagining simultaneously all the possible movements corresponding to a particular form of Jacobi's function. If then we retain the classical idea of a particle localised in space and having in consequence a velocity and a path, it is possible to identify the particle with one of the probability elements. In fact, these elements describe the different possible paths of the particle and consequently the particle must continually coincide with one of them.

If now we still wish to retain the classical conception of the particle in the domain proper of the new mechanics, that is to say, outside the approximation to geometrical optics, we naturally wish to maintain the identity of the particle with one of the probability elements and to represent the state of affairs by imagining on the one hand the wave, and on the other the particle to be localised in space, and we connect the motion of the particle with the propagation of the wave by the relation :

$$\mathbf{v} = -\frac{1}{m} \text{grad } \phi, \quad . \quad . \quad . \quad (38)$$

where  $\phi$  is the phase of the wave defined by (32). The velocity of the particle is thus determined at each instant if we know the initial position, and thus its path also is determined. Moreover, from the formulæ of the first paragraph, if we know the form of the associated  $\psi$ -wave and if we know that initially the probability of occurrence of the particle at a point is equal to the intensity of the wave at the point, it will be so automatically at every succeeding instant ; thus the principle of interference will be satisfied. We may describe this theory as the pilot-wave theory, because we imagine the wave as guiding the motion of the particle.

This theory may at first sight appear satisfactory because it allows the retention of the classical conception of the particle while being in agreement with the principle of interference. But on closer examination it is seen to raise serious objections which we will briefly consider.

One fundamental difficulty comes from the fact that in the domain of the new dynamics the determination of the function  $\phi$  is not independent of that of the determination of  $a$ . If, therefore, we suppose the motion of the particles to be given by (38), this motion will depend not only on the initial position but also on the probability of this initial position, since it depends upon  $a(x, y, z, 0)$ . This is a wider deviation at the outset from classical ideas than is apparent at first sight, for according to these ideas it is inconceivable that the order of accuracy of our knowledge of the initial state can influence the later course of the motion.

Moreover, from the moment when we accept the principle of interference in complete generality, it becomes very difficult to retain for the wave the character of a physical phenomenon in the old sense of the term. For example, let us consider a particle and its associated wave incident upon an imperfectly reflecting mirror; one part of the wave is transmitted through the mirror, another part is reflected. On account of the meaning attributed to the intensity of the wave, this division of the incident wave into transmitted and reflected waves means that the particle has a certain probability of going through the mirror and a certain probability of being turned back.

Let us suppose that an experiment has just revealed the presence of the particle in the transmitted beam, then the probability of finding it in the reflected beam is zero, and this beam must from now have zero intensity; the experiment on the transmitted beam causes the reflected one to vanish. This seems to be a necessary consequence of the interference principle applied to the case of a single particle, and it is difficult to conclude otherwise than that the wave is not a physical phenomenon in the old sense of the word. It is of the nature of a symbolic representation of a probability in space and time, but the idea of a particle guided by the wave then becomes less satisfactory. So long as it was possible to regard the wave as a physical phenomenon, it was easy to adopt the view that it could guide the particle in its motion. But if the wave is

merely a symbolic representation of a probability, the guidance of the particle by the wave becomes much more difficult to understand and much less in harmony with the old ideas of mechanics.

We have seen that in general there is neither conservation of energy nor of momentum for the probability elements, even in the absence of a field. This is clearly also the case for the particle if its motion is identified with that of one of the probability elements, and this results in the loss of a great part of the utility of the pilot-wave theory. Let us consider, for example, the case in which the external field is zero and in which the wave is a superposition of plane monochromatic waves. In the pilot-wave theory the energy and momentum of the particle at the point  $(x, y, z)$  at time  $t$  would be found by calculating  $\frac{\partial \phi}{\partial t}$  and  $-\text{grad } \phi$  for these values of

the variables. This is easily done by means of (37), and it is found that the energy and momentum of the particle would vary in a complicated way in the course of time and would depend, moreover, on the form of the wave-train; the motion of the particle thus deduced seems hardly likely to be the correct one. Moreover, there are reasons for thinking that if we sought to measure in this case the energy of the particle we should find one or other of the values corresponding to the frequencies of the plane monochromatic waves which make up the wave-train, and not the value given by  $\frac{\partial \phi}{\partial t}$ . We shall return

to this important point in the next chapter, where we shall be occupied with the case of light, and we shall see that herein lies one of the essential differences between the pilot-wave theory and the point of view of Bohr and Heisenberg. In short, the pilot-wave theory which localises the particle at a point of the wave, attributing to it a well-defined motion at each point, finds itself confronted with serious difficulties.

But there is no inconvenience—on the contrary there are advantages from the point of view of visual representation—in retaining the picture of the probability cloud, the elements of which possess motion defined by (5) and of which the density, equal to the intensity of the associated wave, measures at each point of space and time the probability of occurrence of the particle in agreement with the principle of interference.



## CHAPTER X

### THE WAVE MECHANICS OF LIGHT QUANTA

#### 1. Photons and their Associated Waves

**I**N the present chapter we shall develop the conception of the probability cloud for light quanta. But as the demonstrations of the preceding chapter have been made by utilising the non-relativistic equations, we shall be obliged to go over them again, since there can be no question of applying non-relativistic equations to the motion of photons.

We have for the relativistic equation for the wave associated with a particle when there is no field of force :

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \frac{4\pi^2 m^2 c^2}{h^2} \psi. \quad . \quad . \quad (1)$$

Introducing the notation :

$$\square^2 = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}, \quad . \quad . \quad (2)$$

we may rewrite (1) thus :

$$\square^2 \psi = \frac{4\pi^2 m^2 c^2}{h^2} \psi. \quad . \quad . \quad (3)$$

A solution of this equation of a simple sinusoidal form corresponding to rectilinear uniform motion is :

$$\psi = ae^{\frac{2\pi i}{h}\{Wt - (p_x x + p_y y + p_z z)\}}. \quad . \quad . \quad (4)$$

the energy  $W$  of the particle and its momentum  $\mathbf{p}$  being expressed as a function of the mass  $m$  and of the velocity by the relativity formulæ :

$$W = \frac{mc^2}{\sqrt{1 - \beta^2}}, \quad \mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1 - \beta^2}}. \quad . \quad . \quad (5)$$

Remembering this, let us consider a succession of particles of smaller and smaller proper masses. Simple sinusoidal solutions will always exist of the type (4) corresponding to a given value  $W$  of the energy, but in proportion as the mass  $m$  tends to zero, the velocity  $v$  tends to  $c$ , since  $W$  is kept constant. In passing to the limit we can conceive particles of mass zero the waves of which will have the frequency  $\nu = \frac{W}{h}$  and of which the velocity is  $c$ . It suffices to suppose that  $m$  and  $\beta$  tend simultaneously the one to zero and the other to unity, so that the ratio  $\frac{mc^2}{\sqrt{1-\beta^2}}$  preserves the same value  $h\nu$ . For these particles of zero mass we have therefore :

$$W = h\nu, \quad p = \text{Lim} \frac{mv}{\sqrt{1-\beta^2}} = \frac{h\nu}{c} \quad . \quad . \quad . \quad (6)$$

These are the fundamental relations of Einstein's quantum theory of light, which have made it possible to give an explanation to the photo-electric and to the Compton effect. We are thus led to consider light as made up of particles of zero mass which we shall call photons. The equation of their associated waves is obtained by making  $m = 0$  in equation (3), which gives the classical equation of light waves :

$$\square^2 \psi = 0. \quad . \quad . \quad . \quad . \quad (7)$$

Thus we shall always associate a solution of the wave equation (7) with the photon, and we shall identify this solution with the classical luminous wave. It is, of course, to be understood in the general case that the wave will not be plane and monochromatic, but a general solution of (7).

## 2. The Probability Cloud Associated with a Photon

We still adopt the principle of interference that the intensity of the  $\psi$ -wave must give the probability of occurrence of the associated photon in such a way that in a case where many photons occur this intensity measures the amount of energy which can be received at any point. In this way we are in agreement with the meaning attributed to the intensity of a light wave in classical theories. As in the case of electrons and other material particles, it is natural to assume for the

photons a probability cloud connected with the  $\psi$ -wave so that the interference principle is satisfied.

In order to avoid certain complications we shall suppose that the  $\psi$ -wave consists approximately of a super-position of plane monochromatic waves of the same frequency  $\nu$ , which is the case approximately realised in practice in ordinary experiments in interference. We can then write :

$$\begin{aligned}\psi(x, y, z, t) &= \sum_k a_k e^{2\pi i\nu \left(t - \frac{\alpha_k x + \beta_k y + \gamma_k z}{c}\right)} = ae^{\frac{2\pi i}{h}\phi} \\ &= ae^{\frac{2\pi i}{h}(h\nu t - \phi_1)}.\end{aligned}\quad (8)$$

where  $a$  and  $\phi_1$  are functions of  $(x, y, z)$ .

If we substitute (8) in (7) and separate the real and imaginary parts, we obtain :

$$\frac{h^2 v^2}{c^2} - \sum (\frac{\partial \phi}{\partial x})^2 = - \frac{h^2}{4\pi^2} \frac{\nabla^2 a}{a} \quad (9)$$

$$\sum \frac{\partial \phi}{\partial x} \frac{\partial a}{\partial x} + \frac{1}{2} a \nabla^2 \phi = \frac{h\nu}{c^2} \frac{\partial a}{\partial t}. \quad (10)$$

Equation (10) shows at once that if we attribute to the probability elements the velocity :

$$\mathbf{v} = -\frac{c^2}{h\nu} \text{grad } \phi, \quad (11)$$

the interference principle will be satisfied. We may, in fact, by using (11) and writing  $a^2 = \rho$ , write (10) in the form :

$$\operatorname{div}(\rho \mathbf{v}) + \frac{\partial \rho}{\partial t} = 0. \quad (12)$$

This is the equation of continuity for the motion of the probability fluid if we suppose, as the interference principle requires, that  $\rho$  is the probability density.

Equation (11) suggests the definition of the momentum and energy of the probability elements by means of :

$$\mathbf{p} = -\text{grad } \phi, \quad W = \frac{\partial \phi}{\partial t} = h\nu, \quad . \quad . \quad (13)$$

for then  $p = \frac{h\nu}{c^2} = \frac{Wv}{c^2}$ , and we again obtain the formula which relates energy and momentum in relativistic dynamics. If we

adopt the definitions of (13), equation (9) appears as the Jacobi equation of the probability elements.

It is easy to write down the equations of motion of these elements, for :

$$\begin{aligned}\frac{dp_x}{dt} &= \frac{\partial p_x}{\partial x} v_x + \frac{\partial p_x}{\partial y} v_y + \frac{\partial p_x}{\partial z} v_z + \frac{\partial p_x}{\partial t} \\ &= \frac{c^2}{h\nu} \left( \frac{\partial \phi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial \phi}{\partial y} \frac{\partial^2 \phi}{\partial x \partial y} + \frac{\partial \phi}{\partial z} \frac{\partial^2 \phi}{\partial x \partial z} \right) = \frac{c^2}{2h\nu} \frac{\partial}{\partial x} \left\{ \sum \left( \frac{\partial \phi}{\partial x} \right)^2 \right\}\end{aligned}\quad (14)$$

Whence by (9) :

$$\frac{dp_x}{dt} = \frac{hc^2}{8\pi^2\nu} \frac{\partial}{\partial x} \left( \frac{\nabla^2 a}{a} \right) = - \frac{\partial F_1}{\partial x}, \quad (15)$$

writing  $F_1 = - \frac{hc^2}{8\pi^2\nu} \frac{\nabla^2 a}{a}$ , and there are similar equations for  $p_y$  and  $p_z$ . These three equations determine the motion of the elements as a function of  $a$  and  $\phi$  and the derivatives of  $F_1$  may be described as the components of the quantum force derived from the quantum potential  $F_1$ . It is, of course, clear that in general the quantities ( $p_x$ ,  $p_y$ ,  $p_z$ ) are not constant; in general the momentum is not conserved in the case of the probability elements, because the quantum force does not always vanish.

### 3. Interpretation of Interference Phenomena

When the wave-train is very long and no obstacle lies in its path, we can represent it by a plane monochromatic wave :

$$\psi = ae^{2\pi i \left\{ vt - \frac{\nu}{c}(\alpha x + \beta y + \gamma z) \right\}} \quad (18)$$

and the phase is thus :

$$\phi = hvt - \frac{h\nu}{c}(\alpha x + \beta y + \gamma z). \quad (19)$$

The probability elements have then all the same velocity along the direction ( $\alpha$ ,  $\beta$ ,  $\gamma$ ) and equal to :

$$v = - \frac{c^2}{h\nu} \left| \text{grad } \phi \right| = c. \quad (20)$$

If we consider a large number of photons with associated waves all of the form (18), from the statistical point of view it

is as if the photons described rectilinear paths with velocity  $c$ , so that we have again the linear propagation of light.

This is no longer the case when the wave encounters obstacles (mirrors, screens, etc.). The mathematical form of the wave must then be modified so as to satisfy certain conditions at the boundaries and the phenomena of interference and diffraction occur.

If we suppose that the obstacles encountered by the wave are fixed, there is no modification of the incident frequency, and it will always be possible to express the wave in the complex form :

$$\psi = ae^{\frac{2\pi i}{h}(h\nu t - \phi_1)} \quad . \quad . \quad . \quad (21)$$

The phase is a linear function in the time, and  $a$  and  $\phi_1$  are functions of  $(x, y, z)$  only. Equation (11) can be written in this case :

$$\mathbf{v} = \frac{c^2}{h\nu} \text{grad } \phi_1, \quad . \quad . \quad . \quad (22)$$

and determines the motion of the probability elements in the region where interference is taking place. The probability of occurrence of the photon in an element of volume  $dv$  is :

$$Pdv = a^2 dv, \quad . \quad . \quad . \quad (23)$$

the constant factor of  $a$  being suitably chosen.

Formula (23) makes it possible to obtain once more the explanation of the phenomena of interference and diffraction of light given by classical theories. In fact, it states that if we consider an assembly of photons associated with identical waves the number of photons passing per second at the site of interference phenomena is proportional to the intensity of the wave at this point. Thus by comparing, as it is natural to do, the  $\psi$ -wave of the photons with the classical light wave, the new mechanics leads us to anticipate the same system of bright and dark fringes as the classical theory.

In order to record interference fringes, for example by photography, we can make an experiment of short duration with intense illumination or one of long duration with feeble illumination ; in the former case we take an average in space, in the latter an average in time, but the result must evidently be the same. This explains why experiments on interference and

diffraction are independent of the intensity. We must lay further stress upon this important point. Let us consider an experiment in which interference is obtained with very feeble illumination and a very long exposure. From time to time the source emits a photon, and these emissions are so widely separated from one another that in general there is only a single photon with its associated wave-train crossing the interference apparatus. The probability that the presence of the photon will be made known by photographic action in the apparatus is everywhere proportional to the resultant intensity of the wave-train. During the very long duration of the experiment, the process of emission is repeated a very great number of times,  $N$ , and the apparatus receives in succession  $N$  identical wave-trains.

Clearly the photographic effect produced is the same as if the apparatus had received a single wave-train carrying  $N$  photons distributed in the train in proportion to the square of the amplitude. Thus the experiment made with very feeble illumination and very long duration must give the same result in agreement with classical theory as a rapid experiment with intense illumination. It is almost certain that the same considerations are valid for the diffraction of material particles.

Equations (15) for the motion of the probability show that in a case where there is interference in the presence of fixed obstacles the probability elements do not move in a straight line; their path is curved by the action of the quantum force which itself results from the variation of amplitude. Let us take the simple example of the diffraction of a plane wave by the straight edge of a plane semi-infinite screen. The light penetrates the geometric shadow, as is known from Fresnel's principle. Thus there are necessarily probability elements which bend round the edge of the screen and clearly there is not conservation of momentum in the ordinary sense. This suggests a remark of interest from the historical point of view. The supporters of Newton's corpuscular theory formerly held after the discovery of this phenomenon that the edge of a screen exerted a force on the light corpuscles; we return to some extent to this view with our quantum force, which is indeed a consequence of the presence of the screen. But the quantum force is of a very special character and without the adoption

of the pilot-wave theory, of which we know already the difficulties, we cannot consider the quantum force correctly described as applied to the particle itself.

#### 4. The Interference of Light in the Neighbourhood of a Perfectly Reflecting Plane Mirror

It is very instructive to study the probability motion in a special case of interference; that which occurs in the neighbourhood of a plane mirror struck by a beam of light. We shall take first the case of a perfectly reflecting plane mirror, the plane of the mirror being taken as that of  $xy$ , the plane of

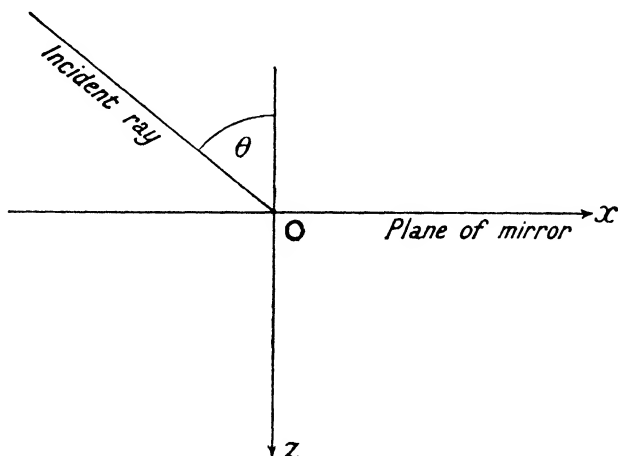


FIG. 7.

incidence or plane of the figure as  $zx$ , and the axis of  $z$  will be the normal to the mirror directed away from the incident wave.

The incident plane wave is :

$$\psi_1 = a_0 e^{2\pi i v \left( t - \frac{x \sin \theta + z \cos \theta}{c} \right)} \quad . \quad . \quad . \quad (24)$$

and the reflected wave :

$$\psi_2 = a_0 e^{2\pi i v \left( t - \frac{x \sin \theta - z \cos \theta}{c} + \alpha \right)} \quad , \quad . \quad . \quad (25)$$

the amplitude is the same in both cases because the mirror is perfectly reflecting, and  $\alpha$  is a constant corresponding to a possible change of phase occurring on reflection.

Near the mirror there is superposition of the waves  $\psi_1$  and  $\psi_2$  and we have :

$$\psi = \psi_1 + \psi_2 = ae^{\frac{2\pi i}{h}\phi}, \quad . \quad . \quad (26)$$

where

$$a = 2a_0 \cos \left( 2\pi \frac{\nu}{c} z \cos \theta + \frac{\alpha}{2} \right), \quad . \quad . \quad (27)$$

$$\phi = h\nu \left( t - \frac{x \sin \theta}{c} \right) + \frac{h\alpha}{4\pi}. \quad . \quad . \quad (28)$$

According to (11) the velocity of the probability elements in the interference region has components :

$$v_x = -\frac{c^2}{h\nu} \frac{\partial \phi}{\partial x} = c \sin \theta, \quad v_y = v_z = 0. \quad . \quad (29)$$

Thus in the neighbourhood of the mirror the probability moves parallel to it and its density,  $a^2$ , has maxima and minima on planes parallel to the reflecting surface with a separation of magnitude  $\frac{\lambda}{4 \cos \theta}$  by (27). The probability fluid, homogeneous in the incident beam where all positions of the photon are equally probable, divides itself into parallel layers on entering the region of interference. We are, of course, in practice always concerned with limited trains of waves presenting a wave front, and the motion of the probability which we have just described exists only when, the wave front having been reflected by the mirror, the interference system is established.

In the example we have just studied we may be tempted to say that the probability tracks are actually the paths of the photons themselves ; this is the point of view of the pilot-wave theory. The photons uniformly distributed in the incident wave would come into the interference region and form layers which would flow parallel to the surface of the mirror. But, as we have seen, this identification of the motion of the corpuscles with that of the probability elements raises difficulties of principle. When we pass on to consider the case of an imperfectly reflecting mirror we shall see that the pilot-wave theory leads to an improbable result on the subject of the velocity of the photons.



### 5. The Interference of Light in the Neighbourhood of an Imperfectly Reflecting Plane Mirror

We pass on to the case of a plane mirror which is not perfectly reflecting. Some of the photons will be transmitted through the surface of the mirror into the medium situated behind, while the rest will be reflected. We shall consider the surface of the mirror as a very thin transition layer in which the partial reflection of the wave takes place.

It is of little importance for what follows whether the medium behind this layer is identical with the medium (air or vacuum) situated on the side of incidence or consists, on the contrary, of a refracting body. On the side of incidence there is a region where the superposition of the incident and reflected waves gives rise to interference. We wish to understand how the probability elements are to traverse this region of interference in order that some may enter into the reflected, others into the transmitted, beam.

The incident wave  $\psi_1$  is still given by (24), but in order to simplify the calculation somewhat we will take  $a_0 = 1$ . It would be quite easy to restore  $a_0$  and  $a_0^2$  to all the formulæ. We shall thus write :

$$\psi_1 = e^{\frac{2\pi i\nu}{c}\left(t - \frac{x \sin \theta + z \cos \theta}{c}\right)} \quad . \quad . \quad (30)$$

for the incident wave and

$$\psi_2 = \eta e^{\frac{2\pi i\nu}{c}\left(t - \frac{x \sin \theta - z \cos \theta}{c}\right) + \alpha} \quad . \quad . \quad (31)$$

for the reflected wave.

If  $\eta = 1$ , the mirror is perfectly reflecting and we again have the problem considered above. If  $\eta = 0$  the beam is transmitted without any reflection, or the mirror does not exist. In the intermediate case,  $0 < \eta < 1$ , the proportion of the probability elements which undergo reflection is  $\eta^2$  by the interference principle. At the site of interference in the neighbourhood of the mirror on the side of incidence, the resultant wave is :

$$\psi = \psi_1 + \psi_2 = ae^{\frac{2\pi i}{h}\phi} \quad . \quad . \quad (32)$$

For the sake of brevity write :

$$\mu = \frac{4\pi\nu}{c} z \cos \theta + \alpha.$$

To determine  $a$  and  $\phi$  we make use of (35) and (37) of the preceding chapter, and we find easily :

$$\left. \begin{aligned} a^2 &= 1 + \eta^2 + 2\eta \cos \mu \\ \frac{\partial \phi}{\partial x} &= -\frac{h\nu}{c} \sin \theta, \quad \frac{\partial \phi}{\partial y} = 0, \quad \frac{\partial \phi}{\partial z} = -\frac{h\nu}{c} \cos \theta \frac{1 - \eta^2}{a^2}, \end{aligned} \right\} \quad (33)$$

The velocity components of the probability elements are by (11) :

$$v_x = c \sin \theta, \quad v_y = 0, \quad v_z = c \cos \theta \frac{1 - \eta^2}{a^2}. \quad (34)$$

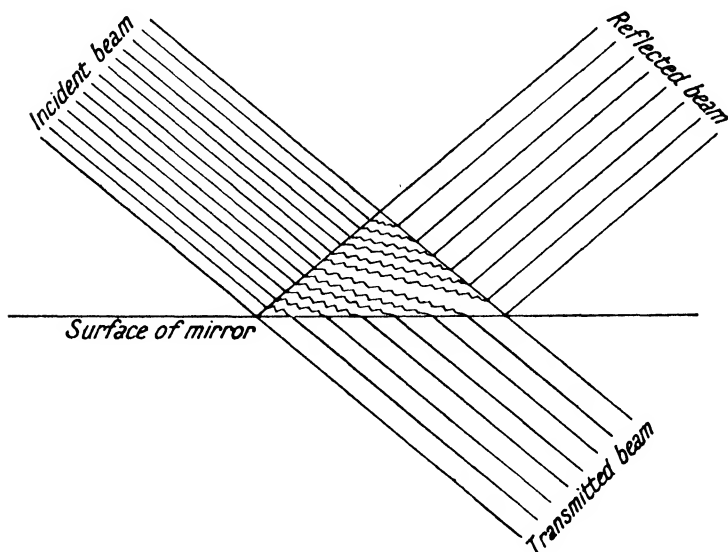


FIG. 8.

The motion of the probability elements is thus in the plane of incidence, and their velocity parallel to the mirror is the same as if the latter were perfectly reflecting. But in this case  $v_z$  is no longer zero, it is a periodic function of  $z$ , and we conclude that the probability tracks in the interference region are wavy curves similar to those of Fig. 8. It is easily seen that the average slope of these wavy curves lies between the value 0 corresponding to the case where  $\eta = 1$ , which has already been considered, and the value  $\tan \theta$  corresponding to the case of total transmission,  $\eta = 0$ .

In Fig. 8 it is seen how the probability elements uniformly

distributed in the incident bundle come to occupy some the transmitted and others the reflected beam, the density of their redistribution in these two bundles being again uniform. In the interference region the probability density is given by the value of  $a^2$  in equation (33). Thus there are in this case bright and dark fringes parallel to the surface of the mirror, but the dark fringes are not absolutely black, since the minima of  $a^2$  are equal to  $(1 - \eta)^2$  which is always positive. Thus in the interference region there is no place where no probability element exists. These conclusions are almost evident from Fig. 8, for if the dark fringes were quite black it would be difficult to see how the probability elements would come to occupy the transmitted beam.

Here again it is tempting to imagine the photons as localised points describing probability paths. But apart from the difficulties already mentioned, another very interesting one arises here. If we examine (34) we see that the component  $v_z$  is greater than  $c \cos \theta$  in the dark fringes. The result is that in these fringes the velocity  $v$  of the probability elements is greater than  $c$  for :

$$v^2 = v_x^2 + v_y^2 + v_z^2 = c^2 \sin^2 \theta + c^2 \cos^2 \theta \left( \frac{1 + \eta}{1 - \eta} \right)^2 > c^2, \quad (35)$$

so that if we wish to attribute the probability motion to the photons we are compelled to attribute to them a velocity greater than  $c$  in the dark fringes, and this would be very difficult to reconcile with the principle of relativity.

## 6. The Superposition of Two Plane Monochromatic Waves

Let us consider a light wave formed by superposing two plane monochromatic waves travelling in the direction of  $z$  :

$$\psi = a_1 e^{\frac{2\pi i \nu_1}{c} \left( t - \frac{z}{c} \right)} + a_2 e^{\frac{2\pi i \nu_2}{c} \left( t - \frac{z}{c} \right)}. \quad (36)$$

If we write  $\psi$  in the form  $ae^{\frac{2\pi i}{h}\phi}$  we find :

$$a^2 = a_1^2 + a_2^2 + 2a_1 a_2 \cos 2\pi(\nu_1 - \nu_2) \left( t - \frac{z}{c} \right), \quad (37)$$

and thus there are maxima and minima travelling along the  $z$ -axis at space intervals of magnitude  $\frac{c}{\nu_1 - \nu_2}$ . The probability

of occurrence of the associated photon must be equal to  $a^2$  by the interference principle, and thus has the same maxima and minima.

If we calculate the quantity  $\frac{\partial\phi}{\partial t}$ , which plays the part of energy for the elements, we find :

$$\begin{aligned} \frac{\partial\phi}{\partial t} &= \frac{h}{4\pi i} \cdot \frac{1}{a^2} \left( \psi^* \frac{\partial\psi}{\partial t} - \psi \frac{\partial\psi^*}{\partial t} \right) \\ &= \frac{a_1^2 h\nu_1 + a_2^2 h\nu_2 + a_1 a_2 (h\nu_1 + h\nu_2) \cos 2\pi(\nu_1 - \nu_2) \left( t - \frac{z}{c} \right)}{a_1^2 + a_2^2 + 2a_1 a_2 \cos 2\pi(\nu_1 - \nu_2) \left( t - \frac{z}{c} \right)}. \end{aligned}$$

If  $\nu_1 = \nu_2 = \nu$ , we find, of course, the constant value  $h\nu$  for  $\frac{\partial\phi}{\partial t}$ , but in the general case  $\nu_1 \neq \nu_2$ ,  $\frac{\partial\phi}{\partial t}$  is a complicated variable quantity. In the pilot-wave theory, where we attempt to identify the motion of the particle with that of the probability elements, the particle ought to have this continually varying energy  $\frac{\partial\phi}{\partial t}$ . Now it appears certain that if we allow the wave (36) to fall on a piece of matter, we obtain a photo-electric effect corresponding either to the quantum  $h\nu_1$  or to the quantum  $h\nu_2$ . Everything takes place as if the associated particle had either the energy  $h\nu_1$  or  $h\nu_2$ , but not the energy  $\frac{\partial\phi}{\partial t}$ . Thus to obtain the probability of occurrence of the particle we must consider the amplitude  $a$  resulting from the superposition of two monochromatic waves. On the other hand, to anticipate the different amounts of energy with which the particle can appear, we must consider not the resulting phase but the frequencies of the different monochromatic waves, that is to say, the spectral distribution of the  $\psi$ -wave. There are thus several possibilities—in our example there are two—for the value of the energy of the particle. We can no longer attribute a definite energy to the particle as does the pilot-wave theory, but only speak of the probability that it will appear with so much energy.

Similar considerations can be applied to the momentum.

## CHAPTER XI

### THE THEORY OF BOHR AND HEISENBERG

#### 1. The Principle of Spectral Distribution

TO sum up the results obtained to this point: we have seen that it is always necessary to associate with the motion of a particle the propagation of a wave  $\psi = ae^{\frac{2\pi i}{h}\phi}$  and that an essential principle, necessary for the interpretation of experimental results, is the interference principle according to which the resultant intensity of the wave,  $a^2 = \psi\psi^*$ , measures always and everywhere, in the case both of matter and light, the probability of occurrence of the particle. Moreover, we were led to imagine a fictitious fluid or probability fluid, the motion of which is determined by the propagation of the wave and the density  $a^2$  of which gives the probability of occurrence according to the interference principle. The motion of the elements of the probability fluid coincides with the possible motion of the particle as described by the old dynamics when the approximations of geometrical optics are applicable to the study of the wave. We were therefore led to suppose that the particles are well-defined points describing probability paths, but examination of this point of view (the pilot-wave theory) revealed difficulties. Thus the true meaning of the duality of waves and particles still remains obscure, and we can now conveniently pass on to the theory of Bohr and Heisenberg.

This theory rests on two principles. Firstly, the interference principle which we know already; and secondly, the principle of spectral distribution, to which we were introduced at the end of the last chapter, and which we will explain more fully by a consideration of the case of the zero field. The starting-point of wave mechanics is that a plane monochromatic

wave corresponds to the uniform rectilinear motion of a particle. But a limited wave-train can be considered as a superposition of plane monochromatic waves of the form :

$$\psi = \sum_k a_k \psi_k = \sum_k a_k e^{2\pi i \nu_k \left\{ t - \frac{n_k}{c} (\alpha_k x + \beta_k y + \gamma_k z) \right\}}, \quad (1)$$

the constants  $\alpha_k$ ,  $\beta_k$ ,  $\gamma_k$ , and  $n_k$  being related by the equations :

$$\alpha_k^2 + \beta_k^2 + \gamma_k^2 = 1, \quad n_k = \sqrt{1 - \frac{\nu_0^2}{\nu_k^2}}, \quad (2)$$

where  $\nu_0$  is the proper frequency  $\frac{mc^2}{h}$  of the particle.

From the beginning of the development of wave mechanics Born has proposed to consider each quantity  $a_k^2$  as giving the relative probability that the particle possesses the state of motion corresponding to  $\psi_k$ .

Thus, contrary to the view of the pilot-wave theory, the  $\psi$ -wave would not give the motion of the particle but only the probability that it has this or that state of motion. With Born's hypothesis, the difficulties pointed out at the end of the last chapter with regard to the photo-electric effects produced by a wave, which is the superposition of two or more monochromatic waves, disappear spontaneously. We shall describe Born's postulate as the principle of spectral distribution. If we accept it the definition of the particle by its associated wave is subject to a double uncertainty ; on the one hand, its position is uncertain by the interference principle, since there is a certain probability measured by  $a^2$  that the particle may be found at any point of the region occupied by the wave-train ; on the other hand, the state of motion of the particle defined by its energy and momentum is also uncertain by the principle of spectral distribution, since there are several possible states of motion, the probability of each being given by the square of the amplitude of the corresponding monochromatic component in the spectrum of the wave-train.

How must this double uncertainty be explained ? It is this explanation which the theory of Bohr and Heisenberg attempts to offer by a subtle and profound analysis of the concepts of observation and of measurement.

## 2. The Theory of Bohr and Heisenberg. The Uncertainty Relations

To make an observation on a phenomenon is in some measure to disturb it. We can in fact observe only the establishment of an interaction between the phenomenon studied and the surrounding medium of which the observer himself is a part. If the measuring process disturbs the phenomenon to a relatively small extent, the value of the quantities characteristic of the phenomenon can be regarded as accurately known after the measurement, taking account, of course, of the experimental errors. But if the process changes the phenomenon to a great extent then the result of observation gives no longer any exact information of the state existing after measurement. This state is affected by an uncertainty arising from the lack of knowledge of the way in which the measurement has disturbed the phenomenon. In particular, we may very readily admit that the process of measuring a quantity  $A$  necessarily disturbs the value of a quantity  $B$  in such a way that if the process is improved in order to determine  $A$  more and more accurately, the value of  $B$  afterwards is more and more inaccurately known. The state of a particle is defined according to classical ideas by eight quantities,  $x, y, z, t, p_x, p_y, p_z$ , and  $W$ , which give the position and state of motion at a particular instant. These eight quantities form two groups, the co-ordinates of space and time,  $x, y, z, t$ , and the conjugate quantities of these co-ordinates,  $p_x, p_y, p_z, W$ . We shall show that if the principles of interference and of spectral distribution be accepted any process which measures one of the eight quantities must of necessity alter the value of the conjugate, this change being the greater the more accurately the measurement is made. The uncertainty which results must not be considered as an accidental uncertainty due to an imperfection in our methods of measurement and which could be avoided by improved methods. On the contrary, the uncertainty is an essential one, arising from the disturbance of the phenomenon studied by the act of measurement itself and a consequence of an important natural law.

To show the necessity of this uncertainty as a consequence of the acceptance of the two principles of interference and of

spectral distribution, we will begin by remarking that it must always be possible to represent the result of an observation on a particle by a wave-train. The extension of the wave-train in space represents the uncertainty about the position of the particle after the observation and the extension in the spectral domain occupied by the frequencies of the simple sinusoidal waves which superimpose to form the wave-train corresponds to the uncertainty about the state of motion.

According to the fundamental ideas of wave mechanics, the state of uniform rectilinear motion of the particle must be associated with the propagation of a plane monochromatic wave of frequency  $\nu = \frac{W}{h}$  and of wave-length  $\lambda = \frac{h}{p}$ ,  $W$  and  $p$  denoting the energy and momentum of the particle.

Let us introduce the vector  $\mathbf{n}$ , the vector wave-number of the plane monochromatic wave, with the direction of  $\mathbf{p}$  and equal in magnitude to  $\frac{1}{\lambda}$ . We then have :

$$\nu = \frac{W}{h}, \quad N_x = \frac{p_x}{h}, \quad N_y = \frac{p_y}{h}, \quad N_z = \frac{p_z}{h}. \quad (3)$$

Now, as results from the calculations of Chapter IV, § 3, and as can be demonstrated more generally, a wave-train of dimensions  $\delta x, \delta y, \delta z$  in space and of which the time of passage at a point is  $\delta t$ , requires for its mathematical representation an assembly of plane monochromatic waves for which the components of the vector wave-number and frequency fill at least intervals  $\delta N_x, \delta N_y, \delta N_z$  and  $\delta \nu$  related to  $\delta x, \delta y, \delta z$  and  $\delta t$  by the inequalities :

$$\delta N_x \cdot \delta x \geq 1, \quad \delta N_y \cdot \delta y \geq 1, \quad \delta N_z \cdot \delta z \geq 1, \quad \delta \nu \cdot \delta t \geq 1. \quad (4)$$

As we suppose that a state of uniform rectilinear motion of the particle corresponds to each plane monochromatic wave, we must regard the quantities :

$$\delta W = h\delta \nu, \quad \delta p_x = h\delta N_x, \quad \delta p_y = h\delta N_y, \quad \delta p_z = h\delta N_z. \quad (5)$$

as being the uncertainties in the values of the energy and momentum. The relations then become :

$$\delta p_x \cdot \delta x \geq h, \quad \delta p_y \cdot \delta y \geq h, \quad \delta p_z \cdot \delta z \geq h, \quad \delta W \cdot \delta t \geq h, \quad (6)$$



which are the uncertainty relations of Heisenberg. The less the uncertainty in one of the eight quantities  $x, y, z, t, p_x, p_y, p_z, W$ , the greater that in the conjugate quantity by virtue of the meaning attributed to the wave.

### 3. The Meaning of the Wave in the Theory of Bohr and Heisenberg

We may sum up this question by a consideration of how we can regard the  $\psi$ -wave on the view of Bohr and Heisenberg. Let us suppose that at time  $t_0$  an initial observation has been made which allows us to fix the position and state of motion of the particle within certain limits; we admit that the uncertainty about the conjugate quantities resulting from this observation satisfies Heisenberg's relations (6) in the most favourable case. To represent the results of this first observation, we must form a wave-train of which the resultant intensity at each point is equal to the probability that the particle is at the point and of which the spectral distribution indicates the relative probabilities of the different states of motion of the particle. In order to see as far as possible what may result from this imperfectly known initial state, we must follow the propagation of the wave-train and remember that during the whole of its course the probability of occurrence is always measured at each point by the intensity  $a^2$ , and that the probability of each state of motion is measured by the intensity of the corresponding spectral component. We can therefore predict that if a second observation made later at time  $t$  has just provided new information about the position or state of motion of the particle, there is a certain probability that the corpuscle lies in a particular region of space, and some other probability that it has a certain state of motion. These predictions, which give probabilities and not certainties, are the only ones that we can obtain; according to Bohr and Heisenberg, we seek in vain a representation of the particle as a point describing a well-defined path with a definite velocity.

We can, with Heisenberg, describe the wave-train as a probability packet. We have seen that we can associate a probability cloud with it, the density of the probability fluid thus imagined being equal at each point to the intensity  $a^2$  of a wave-train, and measuring in consequence the probability

of occurrence. The probability elements describe paths which depend on the initial extension of the wave-train, that is upon the initial uncertainty of the position of the particle. That the motion of the probability depends on the knowledge of the initial state raises no difficulty, for the probability of an event depends always on the more or less exact knowledge we have of earlier states.

The study of the propagation of the wave-train allows us to state the probability of the different possible positions of the particle at the time  $t$ . If at this instant we make a new observation to determine the position of the particle, the result must agree with our expectations, but, once made, this observation will in general limit the uncertainty about the position of the particle. If, for example, the wave-train occupies a region  $R$  of space, we know before the observation that the particle must lie within this region, but in general we shall know afterwards that it lies in a region  $R_1$  included in  $R$ . To represent the state of our knowledge after the observation it will thus be necessary to make a reduction of the probability packet in such a way that the wave-train now occupies the region  $R_1$  only. Thus by the mere fact of a new observation a part of the old wave-train suddenly vanishes. This shows, as we have mentioned in the introduction, the abstract and symbolic character of the wave according to this view.

Moreover, a breach appears as a consequence of this theory in the old idea of determinism in physical phenomena, for this idea was based on the possibility of determining exact initial data from which subsequent phenomena could be rigorously deduced by rigorous dynamical laws. The motion of a particle could be inexorably fixed when its initial position and velocity were known. But in the theory of Bohr and Heisenberg it becomes impossible to determine simultaneously with absolute certainty the initial position and velocity of a particle, and consequently it becomes impossible to state that its motion is rigorously determined, for expectations based on a theory of probability can alone be obtained on this question.

#### 4. Agreement with the Old Dynamics

There is nevertheless one important fact that the new theory must explain. For all mechanical phenomena on a large scale

the old conceptions are sufficient, and it cannot be denied that a rigorous determinism appears to exist on our ordinary scale for these phenomena. How is this part to be explained? At the outset we must note that with the new ideas two kinds of uncertainty intervene in practice. The first of these, already admitted by classical theories, is, we may say, accidental, arising from the inevitable imperfection in our methods of measurement, and one which could be indefinitely diminished by a continued improvement in experimental technique. The second is the essential and irreducible uncertainty introduced by Heisenberg's uncertainty relations (6). Now, in the cases where the old mechanical conception is well verified, the accidental is much greater than the essential uncertainty and masks it completely. The result is that events take place practically as if Heisenberg's uncertainty did not exist, that is to say, as if, *except for experimental errors*, all the deterministic conceptions of the old dynamics were exact. But if a continually improved experimental technique were to make it possible to confine the values of the dynamical magnitudes to narrower and narrower limits a point would at last be reached where we should come up against the Heisenberg uncertainty.

We will illustrate this by a numerical example.

Consider the motion along the  $x$ -axis of a small billiard ball weighing a milligramme and of negligible dimensions. To determine the initial state we must find the position of its centre and its velocity. Suppose that we have found the abscissa of the centre to within a thousandth of a millimetre, which would be a good determination. Heisenberg's relation tells us that we shall be unable to know the velocity of the ball at this instant with an uncertainty less than :

$$\delta v = \frac{h}{m\delta x} = \frac{6.55 \times 10^{-27}}{10^{-3} \times 10^{-4}} = 6.55 \times 10^{-20} \text{ cm. per sec.}$$

It is evident that there is no practical method of measurement which would permit of the attainment of this degree of accuracy; the Heisenberg uncertainty will be completely masked by the experimental error, and it will be as if this uncertainty did not exist.

The mathematical agreement between the new mechanics, as conceived by Bohr and Heisenberg, and the old mechanics is,

moreover, shown very elegantly by means of Ehrenfest's theorem (Chap. IX, § 3). We have seen that the old mechanics corresponds to the case where geometrical optics is applicable when the conditions of propagation do not vary appreciably on a scale of the same order as the wave-length. As the wave-length in the usual cases is much smaller than anything we can measure directly, we can imagine a wave-train which occupies a region whose dimensions contain very many wave-lengths and which, nevertheless, can be regarded as a point on our ordinary scale. This wave-train can thus be represented by a wave-group moving approximately with Rayleigh's group velocity; it will form a small probability droplet with dimensions too small for our methods of measurement. The equations which express Ehrenfest's theorem are :

$$m\overline{\gamma_x} = \overline{f_x}, \quad m\overline{\gamma_y} = \overline{f_y}, \quad m\overline{\gamma_z} = \overline{f_z}, \quad . \quad . \quad (7)$$

where, for example,  $\gamma_x$  is the time derivative of the velocity of the probability elements along the  $x$ -axis, and for all the elements of the droplet is equal to  $\frac{dU_x}{dt}$ , where  $U_x$  denotes the group velocity along the  $x$ -axis, and consequently  $\overline{\gamma_x} = \frac{dU_x}{dt}$ .

The approximation of geometrical optics being applicable by hypothesis, the force is approximately constant in all the extent of the wave-train, whence  $\overline{f_x} = f_x$ ,  $f_x$  denoting the  $x$ -component of the force in the small region occupied by the wave-train. The same arguments apply to the  $y$ - and  $z$ -components. We have :

$$m \frac{dU_x}{dt} = f_x, \quad m \frac{dU_y}{dt} = f_y, \quad m \frac{dU_z}{dt} = f_z. \quad . \quad (8)$$

The probability droplet thus moves as a whole, like a material point in a given field of force subject to the old dynamics. Of course, the position of the particle within the wave-train is uncertain, but the dimensions of the train being less than anything we can measure, in practice it is as if the particle had always a definite position and moved in accordance with Newton's equations.

We see with what degree of elegance Ehrenfest's theorem enables us to make the union between the old mechanics and the theory of Bohr and Heisenberg.

### 5. Einstein's Objection. Is the Particle non-Localisable or not Localised ?

A conception so novel as that of Bohr and Heisenberg cannot fail to raise objections. We will consider one of these which was raised by Einstein at the Solvay Congress in Brussels in October, 1927. Let a particle and the associated plane monochromatic wave fall normally on a screen pierced by a circular hole, with a photographic film in the form of a hemisphere of large radius behind it (Fig. 9).

If the hole has sufficiently small dimensions, the wave will be diffracted in passing through it, and will spread in all directions

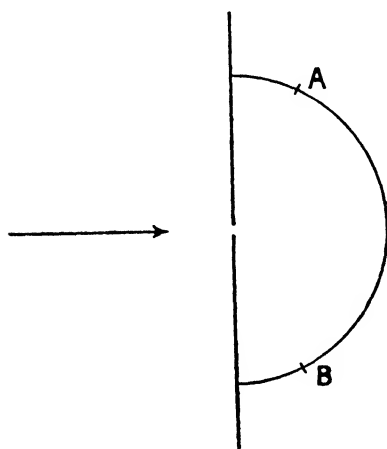


FIG. 9.

to the right of the screen. According to the view of Bohr and Heisenberg, there is a certain probability that the particle will make itself evident by photographic action at some point A of the film. But if a photographic effect is produced at A at the instant  $t$ , no other such effect can be produced anywhere else on the film since there is only one particle present by our hypothesis. Now, with our ordinary ideas of space and

time, even in the relativistic form, it is impossible to understand how the fact that a photographic effect has been produced at A can prevent instantaneously the production of an effect at any other point B unless we admit that the particle is actually localised in space and at each instant occupies a definite point in the associated wave. No other conception appears able to be reconciled with the idea that physical phenomena can be entirely represented in the framework of space and of time, or even in the space-time of Einstein.

This very interesting and simple reasoning of Einstein's shows clearly that we must adopt one or other of the two following attitudes, which we denote by A and B.

(A) We retain the idea that the particle is localised at each instant in space, and that in consequence it has a path and a velocity. We must then express the ideas of Bohr and Heisenberg by saying that although the particle has always a definite position and velocity, an important natural law expressed by Heisenberg's relations (6) prevents us from being able at one and the same time to determine exactly this position and state of motion; for this reason we can only arrive at probabilities with regard to the future positions and states of motion of the particle. From this point of view there is no real indeterminacy, but merely uncertainty imposed by the very nature of things. We should not be able to assert that there is a rigorous determinism in the motion of particles since we could never determine it exactly, but neither could we deny this determinism.

(B) An opinion of a much more radical character, which appears to be held by Bohr and by many other eminent physicists, is that the particle associated with an extended wave-train is not actually localised in space and time; in a certain sense it is present throughout the extent of the wave-train. For Bohr the particles are, in fact, "unsharply defined individuals within finite space-time regions." In Einstein's example the particle would be in some sort virtually spread over the region occupied by the diffracted wave-train; at the moment when the photographic effect is produced at A, the particle would be, as it were, condensed at this point to produce an observable effect. No mechanism in harmony with our ordinary motion of space-time can, so it seems, explain this instantaneous condensation. If we adopt the opinion B, we must say that the space-time frame is insufficient for the complete interpretation of natural phenomena.

Further, the effect produced by the particle always obeys the law of conservation of energy. If, for example, the particle is a photon, the photo-electric effect produced at A will verify Einstein's photo-electric law. It is this property of the particle to condense at a point and produce an effect there in conformity with the causal laws of conservation that Bohr has expressed by saying: "The individuality of the particles transcending the space-time description meets the claim of causality."

At the moment when the particle enters into relation with

the surrounding medium to produce an observable phenomenon, according to the opinion B, it makes, as it were, a choice between several possibilities. Let us consider the reflection on an imperfectly reflecting mirror,  $M$  (Fig. 10).

The incident wave divides into a reflected and a transmitted wave. We must not say that the particle on arriving at the mirror makes a choice between the reflected and transmitted wave, for the arrival of the particle at the mirror is not an observable phenomenon. The transmitted and reflected beams both exist until the instant when the particle manifests its presence in one or the other by an observable phenomenon ;

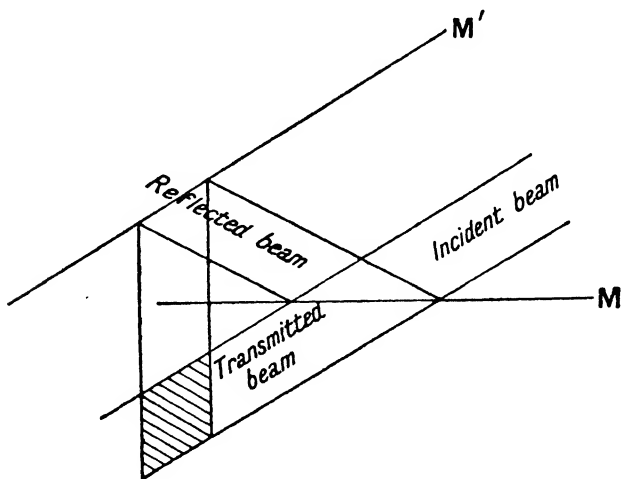


FIG. 10.

only at this moment does the choice operate, for, according to a remark of Heisenberg's, so long as no manifestation of the particle has been produced, interference can be obtained in the shaded parts of Fig. 10 by sending back the reflected beam by means of a mirror  $M'$  on to the transmitted beam, which proves the necessity of considering the two beams.

## 6. Conclusion

These are the broad outlines of the theory of Bohr and Heisenberg on the nature of the reciprocal relation of particles and waves. The theory certainly contains many difficulties

and obscurities. In particular we cannot yet explain in a satisfactory way how it can take account of the experiments of Geiger and Bothe and of those of Compton and Simon which have verified the exactness of the conservation of energy and momentum in individual encounters between photons and electrons.

We must perhaps hope that the introduction of some new idea will help to discover an interpretation of the dualism of waves and particles which will prove more lucid than that proposed by Bohr and Heisenberg.

Nevertheless, it appears certain that there is something fundamental in the uncertainty relations.



## CHAPTER XII

### THE POSSIBILITY OF MEASUREMENT AND HEISENBERG'S RELATIONS

#### 1. Methods of Measurement and Heisenberg's Relations

**T**HROUGHOUT the preceding chapter we have admitted that no observation is capable at one and the same time of determining a co-ordinate and its conjugate momentum with an accuracy greater than that expressed by Heisenberg's uncertainty relations. We must now verify this statement by criticising the methods of measurement at our disposal. This form of criticism was first offered by Heisenberg.

Let us consider a material particle, for example an electron. To determine its position with great accuracy we have only one means, and that is to employ optical methods ; but these allow us to measure a co-ordinate only to an approximation of the order of the wave-length. To increase the accuracy of measurement of the co-ordinates of the particle, we are thus led to employ a shorter and shorter wave-length, but then the particle is subject to a more and more accentuated Compton effect, for the energy of the incident photons is greater and greater and the momentum of the particle is more and more changed by the act of locating it. If, conversely, we propose to measure the velocity and momentum, we shall be able to use the Doppler effect, but this, as we shall see later, is always accompanied by a Compton effect which changes the velocity. To reduce the Compton effect we are led to employ a large wave-length, but then the position of the particles at the instant of measurement will be inaccurately defined.

#### 2. Heisenberg's Microscope

The first illustration of these general considerations is one given by Heisenberg. Let us imagine that an electron in

motion is under examination by a microscope illuminated from below by monochromatic light of frequency  $\nu$  (Fig. 11).

When the electron scatters a photon, a divergent wave enters the microscope. By the well-known theory of the resolving power in classical optics, if the object glass subtends an angle  $2\epsilon$  at the object, a length in the object plane can only be determined with a possible

inaccuracy of  $\frac{\lambda}{2 \sin \epsilon}$  or approximately  $\frac{\lambda}{2\epsilon}$ .

Let the  $y$ -axis lie along the axis of the microscope, which is, of course, the direction of the incident light, and let the  $x$ -axis lie along the direction of the velocity of the electron in the plane of the object carrier. The measurement will only be able to determine the position of the electron on the  $x$ -axis at the instant of scattering with a possible inaccuracy of  $\delta x = \frac{\lambda}{2\epsilon}$ .

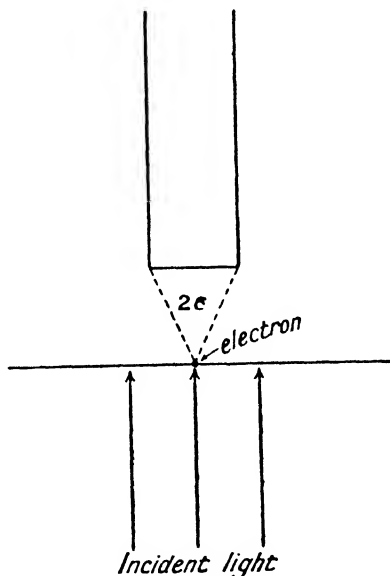


FIG. 11.

Before the scattering, the photon has energy  $h\nu$  and momentum  $\frac{h\nu}{c}$  directed along the  $y$ -axis; the electron has velocity  $\mathbf{v}$  directed along the  $x$ -axis, and if  $v$  is small compared with  $c$ , its momentum is  $m\mathbf{v}$  and its kinetic energy  $\frac{1}{2}mv^2$ . By the Compton effect we know that the scattering modifies the frequency of the photon and the velocity of the electron. After scattering, the photon has frequency  $\nu'$ , energy  $h\nu'$  and momentum  $\frac{h\nu'}{c}$ , making with the axis of the microscope a very small angle  $\alpha$  necessarily less than  $\epsilon$ , since the scattered photon must pass through the objective. The velocity of the electron has become  $\mathbf{v}'$ , its momentum  $m\mathbf{v}'$ , and its energy  $\frac{1}{2}mv'^2$ . Following Compton's method, we shall apply the principles of conservation

of energy and momentum to the process of scattering, and taking  $\alpha^2$  as a small fraction we obtain :

$$\left. \begin{aligned} h\nu + \frac{1}{2}mv_x^2 &= h\nu' + \frac{1}{2}m(v_x'^2 + v_y'^2) \\ \frac{h\nu}{c} &= \frac{h\nu'}{c} + mv_y' \\ mv_x &= \frac{h\nu'}{c}\alpha + mv_x' \end{aligned} \right\} \quad . \quad . \quad . \quad (1)$$

Substituting in the first equation the value of  $\frac{1}{2}m(v_x'^2 + v_y'^2)$  obtained from the other two, we find :

$$\frac{h^2}{mc^2}(\nu - \nu')^2 - 2h(\nu - \nu') - 2\alpha h\nu' \frac{\nu}{c} + \alpha^2 \frac{h^2 \nu'^2}{mc^2} = 0. \quad (2)$$

Equation (2) shows that  $\nu$  differs from  $\nu'$  only by terms of order  $\alpha$ , so that to the first order in  $\alpha$  we may write the last equation of (1) :

$$mv_x - mv_x' = p_x - p_x' = \frac{\alpha h\nu}{c} = \frac{\alpha h}{\lambda}. \quad . \quad . \quad (3)$$

As we do not know the exact value of  $\alpha$  which may vary from  $-\epsilon$  to  $+\epsilon$ , there is an uncertainty in the value of  $p_x$  after scattering of amount :

$$\delta p_x = \frac{2\epsilon h}{\lambda}. \quad . \quad . \quad . \quad (4)$$

Thus, under the most favourable conditions we have :

$$\delta x \times \delta p_x = \frac{\lambda}{2\epsilon} \times \frac{2\epsilon h}{\lambda} = h, \quad . \quad . \quad . \quad (5)$$

and this is Heisenberg's uncertainty relation.

### 3. Measurement of the Velocity of an Electron by Means of the Doppler Effect

We pass on to examine the determination of the velocity of an electron by the Doppler effect. An electron is considered with a velocity  $\mathbf{v}$  along the positive direction of the  $x$ -axis. A train of light waves of average wave-length  $\lambda$  travelling along the negative direction of the  $x$ -axis is projected upon it. If scattering occurs, the scattered photon may undergo a reversal of its velocity and be sent along the positive direction of the

$x$ -axis. Let us suppose that this happens and that we measure the frequency  $\nu'$  of the scattered radiation exactly. For the sake of simplicity, we suppose the velocity of the electron much smaller than that of light. The principles of conservation of energy and momentum give :

$$\left. \begin{aligned} h\nu + \frac{1}{2}mv^2 &= h\nu' + \frac{1}{2}mv'^2 \\ mv - \frac{h\nu}{c} &= mv' + \frac{h\nu'}{c} \end{aligned} \right\}, \quad . \quad . \quad (6)$$

$v'$  being the velocity of the electron after scattering. By elimination of  $v'$  from the equations, we have :

$$h(\nu - \nu') = \frac{1}{2m} \left\{ \frac{h^2}{c^2} (\nu + \nu')^2 - 2mv \frac{h}{c} (\nu + \nu') \right\}. \quad . \quad (7)$$

In the scattering process the frequency is changed very little, and we can thus write :  $\nu' = \nu - \epsilon$ , and neglect  $\epsilon \frac{v}{c}$  and  $\epsilon^2$ .

Hence

$$\epsilon \left( 1 + \frac{2h\nu}{mc^2} \right) = \frac{2h\nu^2}{mc^2} - 2\nu \frac{v}{c}. \quad . \quad . \quad (8)$$

In ordinary cases,  $\frac{h\nu}{mc^2}$  is very small, since for light  $h\nu$  is of the order  $10^{-13}$  and  $mc^2$  is about  $8 \times 10^{-7}$ . We can thus neglect the fraction  $\frac{2h\nu}{mc^2}$  on the left side of (8) and write :

$$\nu' = \nu - \epsilon = \nu \left( 1 - \frac{2h\nu}{mc^2} + 2\frac{v}{c} \right). \quad . \quad . \quad (9)$$

The term  $\frac{2v}{c}$  corresponds to the Doppler effect, and would exist if  $h$  were infinitely small. The term  $-\frac{2h\nu}{mc^2}$  expresses the Compton effect for the case considered and the two effects are superposed. Since the Compton effect alters the velocity of the electron, we must try to make it negligible and take the

wave-length large enough to make the ratio :  $\frac{\frac{v}{c}}{\frac{h\nu}{mc^2}} = \frac{mv}{h} \lambda$  very

large. In this case the Doppler effect alone is appreciable, and we may write :

$$\nu' = \nu \left(1 + \frac{2v}{c}\right) \text{ or } \lambda' = \lambda \left(1 - \frac{2v}{c}\right). \quad (10)$$

But the incident wave-train has necessarily a finite length  $l$ ; consequently it is not strictly monochromatic, and if we introduce the wave-number  $\frac{1}{\lambda}$ , this quantity will vary for the different monochromatic waves of the train by the amount  $\delta\left(\frac{1}{\lambda}\right)$  where :

$$\delta\left(\frac{1}{\lambda}\right) \sim \frac{1}{l} \quad (11)$$

the sign  $\sim$  denoting "of the order of."

Thus, even if  $\lambda'$  be measured without any experimental error, there would still remain an uncertainty in the value of  $v$ , since according to (10) we have :

$$v = \frac{c}{2} \left(1 - \frac{\lambda'}{\lambda}\right), \quad (12)$$

and the uncertainty in  $\lambda$  implies an uncertainty in  $v$  equal to :

$$|\delta v| = \frac{c}{2} \lambda' \delta\left(\frac{1}{\lambda}\right). \quad (13)$$

Thus the uncertainty in the momentum of the electron after measurement is :

$$\delta p_x = \frac{mc\lambda}{2l}. \quad (14)$$

But the simultaneous value of the co-ordinate is itself also subject to an uncertainty.

In fact, the Compton effect, although by hypothesis small in comparison with the Doppler effect, nevertheless exists and causes a change in the velocity of the electron equal by the second of equations (6) to :

$$\begin{aligned} v' - v &= -\frac{h}{mc}(\nu + \nu') \\ &= -\frac{2h}{m\lambda} \text{ (approximately).} \end{aligned} \quad (15)$$

Let us consider the most favourable case, which is that in which the initial position is known. There will be an uncertainty in the position after measurement, since it is not known at what instant in the interval  $\frac{l}{c}$ , during which the wave-train passes the electron, the scattering occurs, and according as this instant is at the beginning or end of the interval there will be a difference  $(v - v')\frac{l}{c} = \frac{2hl}{m\lambda c}$  in the position of the electron. Thus, after the measurement has been made, the co-ordinate of the electron is subject to an uncertainty :

$$\delta x = \frac{2hl}{m\lambda c}, \quad . \quad . \quad . \quad . \quad (16)$$

and combining (14) and (16) we find that in the most favourable case :

$$\delta x \delta p_x = \frac{mc\lambda}{2l} \frac{2hl}{m\lambda c} = h, \quad . \quad . \quad . \quad (17)$$

so that we arrive once more at Heisenberg's uncertainty relation.

#### 4. The Passage of a Particle through a Diaphragm

As another example we will take the determination of the position of a particle, for example a photon, by studying its passage through an opening in a plane screen. In order to fix the co-ordinates of the particle accurately we tend to make the opening very small, but the smaller the opening is made the more pronounced the diffraction phenomena which, according to the ideas of wave mechanics, are associated with the passage of the particle through the hole. Moreover, to find the instant when the particle passes into the plane of the screen we will make use of a movable shutter which will make it possible to uncover the hole for a very short interval. The more rapidly we work the shutter, the better will be the determination of the instant when the particle traverses the hole, but at the same time, the associated wave-train being proportionately shortened, the monochromatic property of the train will be more and more changed and consequently the energy of the particle will be less and less well-defined. We will consider in

detail the simple case where the incident particle falls normally on the screen and where the opening is a rectangle of sides  $2a$  and  $2b$ .

Let the centre of the opening be taken as origin of co-ordinates, the axis of  $x$  being parallel to the longer side  $2a$  and the axis of  $y$  parallel to the shorter side  $2b$ , while the axis of  $z$  is perpendicular to the plane of the screen in the direction away from the incident wave (Fig. 12). Let  $M$  be a point of the opening with co-ordinates  $(X, Y, 0)$ , and let  $(dX, dY)$  be the sides of a small rectangle about this point. Let us determine by Huygen's principle the elementary wave sent by the small

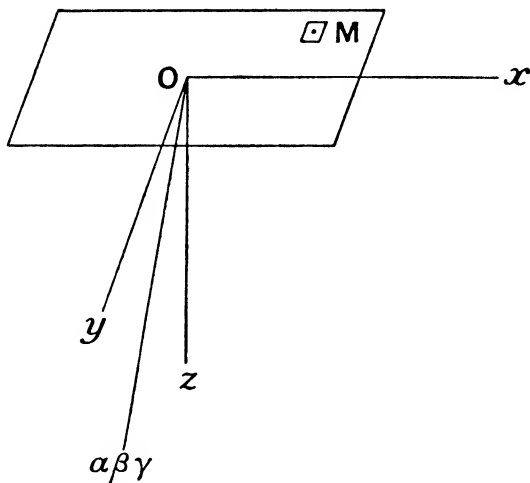


FIG. 12.

rectangle  $dX dY$  in the direction  $(\alpha, \beta, \gamma)$  which makes a very small angle with the  $z$ -axis. If  $(x, y, z)$  denote the co-ordinates of a very distant point in this direction the elementary wave is expressed by :

$$d\psi_{\alpha\beta} = K dX dY \cos 2\pi \left\{ \nu t - \frac{\alpha(x - X) + \beta(y - Y) + z}{\lambda} \right\}, \quad (18)$$

where  $K$  is a coefficient which varies with  $(\alpha, \beta, \gamma)$  but much more slowly than the cosine term and where  $\gamma$  has been written equal to unity. The resulting wave in the direction  $(\alpha, \beta, \gamma)$  from all points of the aperture is

$$\psi_{\alpha\beta} = \iint d\psi_{\alpha\beta} = A \cos 2\pi \left( \nu t - \frac{\alpha x + \beta y + z}{\lambda} \right) + B \sin 2\pi \left( \nu t - \frac{\alpha x + \beta y + z}{\lambda} \right), \quad (19)$$

where

$$A = K \iint \cos 2\pi \frac{\alpha X + \beta Y}{\lambda} dX dY; \quad B = K \iint \sin 2\pi \frac{\alpha X + \beta Y}{\lambda} dX dY. \quad (20)$$

B vanishes because in the integral two elements situated symmetrically with respect to O make equal and opposite contributions. In A we can write :

$$\cos 2\pi \frac{\alpha X + \beta Y}{\lambda} = \cos 2\pi \frac{\alpha X}{\lambda} \cos 2\pi \frac{\beta Y}{\lambda} - \sin 2\pi \frac{\alpha X}{\lambda} \sin 2\pi \frac{\beta Y}{\lambda}, \quad (21)$$

and the integral of the product of the sines again vanishes. Thus :

$$A = 4K \left\{ \int_0^a \cos 2\pi \frac{\alpha X}{\lambda} dX \int_0^b \cos 2\pi \frac{\beta Y}{\lambda} dY \right\} = \frac{K\lambda^2}{\pi^2 \alpha \beta} \sin 2\pi \frac{\alpha a}{\lambda} \sin 2\pi \frac{\beta b}{\lambda} \quad (22)$$

whence

$$\psi_{\alpha\beta} = \frac{K\lambda^2}{\pi^2 \alpha \beta} \sin 2\pi \frac{\alpha a}{\lambda} \sin 2\pi \frac{\beta b}{\lambda} \cos 2\pi \left( \nu t - \frac{\alpha x + \beta y + z}{\lambda} \right). \quad (23)$$

Thus  $\psi_{\alpha\beta}$  vanishes in directions for which  $2\pi \frac{\alpha a}{\lambda} = m\pi$  or  $2\pi \frac{\beta b}{\lambda} = n\pi$ , where  $m$  and  $n$  are integers, that is for directions for which  $\alpha = \frac{m\lambda}{2a}$ , or  $\beta = \frac{n\lambda}{2b}$ . On the other hand,  $\psi_{\alpha\beta}$  has maximum values in the directions for which

$$\alpha = (2m + 1) \frac{\lambda}{2a}, \text{ or } \beta = (2n + 1) \frac{\lambda}{2b}.$$

In this way we obtain what is known as a diffraction phenomenon localised at infinity.

To observe it, we shall place a lens of which the optic axis



coincides with the axis of  $z$ . If there were no diffraction, only an image of the rectangular aperture would be observed situated in the focal plane of the lens on the optic axis. But on account of the existence of plane monochromatic waves inclined to the optic axis, a series of other images are also obtained corresponding to the maxima of  $\psi_{\alpha\beta}$ . The intensity of these images decreases rapidly when the order is raised.

In short, the plane wave which falls on the screen is of the form :

$$\psi = a \cos 2\pi\left(\nu t - \frac{z}{\lambda}\right). \quad . \quad . \quad (24)$$

In passing through the rectangular aperture it is transformed into a group of plane waves slightly inclined to the  $z$ -axis and of the form :

$$\psi = \sum a_{\alpha\beta} \cos 2\pi\left(\nu t - \frac{\alpha x + \beta y + z}{\lambda}\right), \quad . \quad (25)$$

the partial amplitudes  $a_{\alpha\beta}$  representing the successive maxima and minima as functions of  $\alpha$  and  $\beta$ . Since the intensity of the successive waves diminishes rapidly we see that the group extension with respect to the variable  $\alpha$  is measured by :

$$\delta\alpha = k_1 \frac{\lambda}{2a} > \frac{\lambda}{2a}, \quad . \quad . \quad . \quad (26)$$

$k_1$  denoting a small integer which corresponds to the highest order of diffraction for which the intensity is appreciable. In the same way the group extension with respect to  $\beta$  will be :

$$\delta\beta = k_2 \frac{\lambda}{2b} > \frac{\lambda}{2b}. \quad . \quad . \quad . \quad (27)$$

If  $\mathbf{N}$  denotes the wave-number vector for the monochromatic wave characterised by the angles  $\alpha$  and  $\beta$  we have :

$$N_x = \frac{\alpha}{\lambda}, \quad N_y = \frac{\beta}{\lambda}, \quad N_z = \frac{1}{\lambda}. \quad . \quad . \quad (28)$$

The greatest variations of  $N_x$  and  $N_y$  in the wave group after passage through the screen are :

$$\delta N_x = \frac{\delta\alpha}{\lambda} = \frac{k_1}{2a}, \quad \delta N_y = \frac{\delta\beta}{\lambda} = \frac{k_2}{2b}. \quad . \quad . \quad (29)$$

We have, therefore, the following relations in orders of magnitude :

$$\delta N_x \gg \frac{1}{2a}, \quad \delta N_y \gg \frac{1}{2b}. \quad . \quad . \quad . \quad (30)$$

Now the position of the particle at the instant of its passage through the rectangular aperture is defined with an uncertainty  $\delta x$  equal to  $2a$  and an uncertainty  $\delta y$  equal to  $2b$ . We have therefore the relations in orders of magnitude :

$$\delta N_x \delta x \gg 1, \quad \delta N_y \delta y \gg 1. \quad . \quad . \quad (31)$$

According to the principle of spectral distribution, the uncertainties in the components  $p_x$  and  $p_y$  of the momentum are connected with the uncertainties  $\delta N_x$  and  $\delta N_y$  by the equations :

$$\delta p_x = h \delta N_x, \quad \delta p_y = h \delta N_y, \quad . \quad . \quad (32)$$

and (31) thus takes the form of Heisenberg's relations :

$$\delta p_x \delta x \gg h, \quad \delta p_y \delta y \gg h. \quad . \quad . \quad (33)$$

Moreover, if we wish to determine the  $z$ -co-ordinate of the particle and the time  $t$  of the passage through the screen, we must employ a movable shutter in the manner explained above. Let  $\tau$  denote the interval during which the shutter is raised. The uncertainty in  $t$  is clearly equal to  $\tau$ , that in  $z$  is  $v\tau$ ,  $v$  denoting the group velocity which we know is equal to that of the particle. Thus :

$$\delta t = \tau, \quad \delta z = v\tau. \quad . \quad . \quad . \quad (34)$$

But in opening the shutter for the time  $\tau$  only, we allow only a limited wave-train to pass through the aperture, and this train is composed of monochromatic waves occupying an interval in the spectrum at least of the order  $\frac{1}{\tau}$ . The corre-

sponding interval in wave-length is such that  $\delta\left(\frac{1}{\lambda}\right) = \frac{\delta\left(\frac{1}{\lambda}\right)}{\delta\nu} \delta\nu$

is of the order  $\frac{1}{v\tau}$  since  $v = \frac{\delta\left(\frac{1}{\lambda}\right)}{\delta\nu}$  by definition. We have then :

$$\delta\nu \gg \frac{1}{\tau}, \quad \delta\left(\frac{1}{\lambda}\right) \gg \frac{1}{v\tau}. \quad . \quad . \quad . \quad (35)$$

Now by the principle of spectral distribution, the uncertainty in the final energy of the particle is  $\hbar\delta\nu$ , and that in the final value of the component  $p_z$  of the momentum is  $\hbar\delta N_z = \hbar\delta\left(\frac{1}{\lambda}\right)$  by (28). We have thus :

$$\delta W \delta t \geq \hbar, \quad \delta p_z \delta z \geq \hbar. \quad . \quad . \quad . \quad (36)$$

These are the other two Heisenberg relations.

### 5. A Note on the Measurement of Velocity

We have just confirmed by means of examples that the processes of measurement which we are able to use all lead to Heisenberg's uncertainty relations. We might, however, be tempted to reason in the following way. It is possible to make an experiment at a time  $t_1$  showing that the particle is situated in the immediate neighbourhood of a point A of space, then at a later time  $t_2$  another experiment showing that it is then in the immediate neighbourhood of another point B. If the time  $t_2 - t_1$  is sufficiently long, we shall obtain a very good value of the velocity by taking :

$$V = \frac{AB}{t_2 - t_1}, \quad . \quad . \quad . \quad (37)$$

and the value of the momentum  $mv$  does not appear in this way to be affected by the Heisenberg uncertainty.

But we must note, in the first place, that if we repeat the same measurement of the velocity under exactly the same conditions we shall obtain each time a different result. In fact, as we shall show rigorously in the next chapter, the wave-train of very small dimensions, which corresponds at the time  $t_1$  to the localisation of the particle near the point A by the first experiment, spreads during its propagation and occupies a large extent at the end of the long interval  $t_2 - t_1$ , when the second experiment is made. By the principle of interference there is a large region of space where the particle can possibly be found and a series of identical experiments would give a series of different points B.

Moreover, and this is an essential point, the velocity  $v$  given by (37) corresponds only to the motion between the instants  $t_1$  and  $t_2$ ; we cannot in any way consider it as the

velocity which the particle possesses *after* the second experiment, since this second localisation near the point B completely disturbs its motion. The velocity is in no sense the initial velocity of the particle after the second observation, consequently it can give no information of what will happen after the time  $t_2$ . We have not been able to determine simultaneously the position and momentum of the particle by our two measurements of its position. The first observation permits us to localise the particle at A at time  $t_1$ , but it gives us no information about its momentum at this instant; the second permits us to localise the particle at B at  $t_2$  and to find the velocity  $\mathbf{v}$  with which the particle would be carried from A to B, but the momentum  $m\mathbf{v}$  is not that which the particle possesses after the observation. We may say, if we wish, that the particle has passed from A to B with velocity  $\mathbf{v}$ , but that does not allow us in any way to *anticipate* exactly the motion of the particle in the interval  $t_2 - t_1$  as the old deterministic dynamics claimed to do, since  $\mathbf{v}$  has a value defined only at the end of the phenomenon to be anticipated.

In the next chapter we shall study by means of calculations the method of measurement of velocity which we have just discussed.

## CHAPTER XIII

### THE PROPAGATION OF A TRAIN OF $\psi$ -WAVES IN THE ABSENCE OF A FIELD OF FORCE AND IN A UNIFORM FIELD

#### 1. Rigorous Solution of the Equation of Propagation in the Absence of a Field of Force

WE pass on to study rigorously the propagation of a  $\psi$ -wave-train when there is no field of force, contenting ourselves with the non-relativistic equations. We must begin with the equation :

$$\nabla^2 \psi = \frac{4\pi i}{h} m \frac{\partial \psi}{\partial t}. \quad (1)$$

This equation has the same form as the classical equation of thermal conductivity, but here the conductivity is represented by an imaginary coefficient. We can use a method of solution exactly like that applied to the thermal equation.

Equation (1) being of the first order in the time, we must know the value of  $\psi(x, y, z, t)$  at an initial instant taken as the zero time in order to determine which integral is to be chosen. The problem before us is therefore to find  $\psi(x, y, z, t)$  when  $\psi(x, y, z, 0)$  is known. We will write  $\psi(x, y, z, 0) = f(x, y, z)$ . The method of solution is to determine a "transformation function"  $T(x, y, z, x_0, y_0, z_0, t)$  of two sets of variables  $x, y, z$  and  $x_0, y_0, z_0$  and of the time such that :

$$\psi(x, y, z, t) = \iiint f(x_0, y_0, z_0) T(x, y, z, x_0, y_0, z_0, t) dx_0, dy_0, dz_0, \quad (2)$$

where the limits of integration are  $-\infty$  to  $+\infty$  (Kennard, Heisenberg). It is necessary that two conditions should be satisfied.

1. The function  $\psi(x, y, z, t)$  defined by (2) must satisfy the

equation (1); this requires that  $T$  considered as a function of  $x, y, z, t$  shall itself satisfy this equation.

2. The function  $\psi$  defined by (2) must reduce to  $f(x, y, z)$  at  $t = 0$ .

We begin by seeking a function  $T$  which is a solution of the wave equation. We have seen in the study of the classical motion of a particle in a zero field of force that the function :

$$S(x, y, z, t, x_0, y_0, z_0) = -\frac{m}{2t}\{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2\}, \quad (3)$$

depending upon the three initial co-ordinates, is a complete integral of Jacobi's equation, and therefore it is possible to determine the motion which transforms the initial co-ordinates  $x_0, y_0, z_0$  at the instant zero to  $x, y, z$  at the instant  $t$ . We can therefore expect the function  $S$  to play an important part in the problem.

But, on the other hand, the function of transformation  $T$  must satisfy the wave-equation; we have :

$$\nabla^2 T = \frac{4\pi i}{h} m \frac{\partial T}{\partial t}, \quad (4)$$

and if we write :

$$T = \text{Re} e^{\frac{2\pi i}{h} S}, \quad (5)$$

where  $R$  and  $S$  are real functions not yet determined, we find by substituting (5) in (4) and separating real and imaginary parts :

$$\frac{1}{2m} \left\{ \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + \left( \frac{\partial S}{\partial z} \right)^2 \right\} = \frac{\partial S}{\partial t} + \frac{h^2}{8\pi^2 m} \frac{\nabla^2 R}{R}, \quad (6)$$

$$\frac{\partial R}{\partial x} \frac{\partial S}{\partial x} + \frac{\partial R}{\partial y} \frac{\partial S}{\partial y} + \frac{\partial R}{\partial z} \frac{\partial S}{\partial z} + \frac{1}{2} R \nabla^2 S = m \frac{\partial R}{\partial t}. \quad (7)$$

Let us take the expression (3) for the function  $S$ . Since (3) satisfies Jacobi's equation :

$$\frac{1}{2m} \sum \left( \frac{\partial S}{\partial x} \right)^2 = \frac{\partial S}{\partial t}, \quad (8)$$

it is necessary that  $\nabla^2 R$  vanish in order that (6) may be satisfied. The simplest hypothesis is thus to suppose that  $R$  does not

depend on the variables  $(x, y, z)$ , but only upon the time  $t$ . With this assumption equation (7) reduces to :

$$\frac{dR}{dt} = \frac{1}{2m} R \nabla^2 S. \quad (9)$$

This equation can be satisfied since the function (3) which we have chosen for  $S$  is a quadratic in  $(x, y, z)$ , so that  $\nabla^2 S$  is a function of  $t$  only. We have :

$$\nabla^2 S = -\frac{m}{2t} \nabla^2 \{\sum (x - x_0)^2\} = -\frac{3m}{t}, \quad (10)$$

and  $R$  is thus given by :

$$\frac{dR}{dt} = -\frac{3}{2t} R \quad (11)$$

or

$$R = Ct^{-\frac{3}{2}}. \quad (12)$$

We thus obtain by (5), (3) and (12) the function  $T$  :

$$T(x, y, z, x_0, y_0, z_0) = \frac{C}{t^{\frac{3}{2}}} e^{-\frac{\pi i m}{\hbar} \sum (x - x_0)^2}. \quad (13)$$

The function

$$\psi(x, y, z, t) = \iiint f(x_0, y_0, z_0) \frac{C}{t^{\frac{3}{2}}} e^{-\frac{\pi i m}{\hbar} \sum (x - x_0)^2} dx_0 dy_0 dz_0 \quad (14)$$

therefore satisfies the wave equation, but it must also reduce to  $f(x, y, z)$  for  $t = 0$ . In order to verify this we make a change in the variables : <sup>1</sup>

$$r_1 = \frac{x_0 - x}{\sqrt{t}}, \quad r_2 = \frac{y_0 - y}{\sqrt{t}}, \quad r_3 = \frac{z_0 - z}{\sqrt{t}}. \quad (15)$$

The triple integral (14) then becomes :

$$\iiint f\{(r_1\sqrt{t} + x), (r_2\sqrt{t} + y), (r_3\sqrt{t} + z)\} \frac{C}{t^{\frac{3}{2}}} e^{-\frac{\pi i m}{\hbar} (r_1^2 + r_2^2 + r_3^2)} \frac{\partial(x_0, y_0, z_0)}{\partial(r_1, r_2, r_3)} dr_1 dr_2 dr_3. \quad (16)$$

<sup>1</sup>The calculation which follows is due to Fourier. The passage to the limit leading to (18) is not quite rigorous but the reasoning may be made quite sound. Reference may be made to "Leçons sur quelques types simples d'équations aux dérivées partielles," by Emile Picard. Gauthier-Villars, Paris, 1927, 2<sup>e</sup> leçon.

But the Jacobian on evaluation gives :

$$\frac{\partial(x_0, y_0, z_0)}{\partial(r_1, r_2, r_3)} = \begin{vmatrix} \sqrt{t} & 0 & 0 \\ 0 & \sqrt{t} & 0 \\ 0 & 0 & \sqrt{t} \end{vmatrix} = t^{\frac{3}{2}}, \quad (17)$$

so that :

$$\psi(x, y, z, t) = C \iiint f e^{-\frac{\pi i m}{h}(r_1^2 + r_2^2 + r_3^2)} dr_1 dr_2 dr_3. \quad (18)$$

If  $t$  be now made to approach zero the value of  $f$  becomes  $f(x, y, z)$  and we have in the limit :

$$\psi(x, y, z, 0) = f(x, y, z) C \int_{-\infty}^{\infty} e^{-\frac{\pi i m}{h} r_1^2} dr_1 \int_{-\infty}^{\infty} e^{-\frac{\pi i m}{h} r_2^2} dr_2 \int_{-\infty}^{\infty} e^{-\frac{\pi i m}{h} r_3^2} dr_3, \quad (19)$$

since, as we mentioned above, the limits of integration are  $-\infty$  and  $+\infty$ . These are well-known integrals, and we have in fact :

$$\int_{-\infty}^{\infty} e^{-\frac{\pi i m}{h} r^2} dr = \sqrt{\frac{h}{i m}}. \quad (20)$$

If the arbitrary constant  $C$  is given the value  $\left(\frac{i m}{h}\right)^{\frac{3}{2}}$ , we then have :

$$\psi(x, y, z, 0) = f(x, y, z), \quad (22)$$

so that finally the function :

$$\psi(x, y, z, t) = \left(\frac{i m}{h t}\right)^{\frac{3}{2}} \iiint f(x_0, y_0, z_0) e^{-\frac{\pi i m}{h t} \{\Sigma(x - x_0)^2\}} dx_0 dy_0 dz_0, \quad (23)$$

the limits of integration being  $-\infty$  and  $+\infty$  for each of the variables, is the solution of the wave-equation (1) which reduces to  $f(x_0, y_0, z_0)$  for  $t = 0$ .

The problem of the propagation of the wave-train associated with a particle is thus solved rigorously.



## 2. The Calculations Applied to a Special Case (Darwin)

In order to work out the results we shall make a special assumption in regard to the form of the initial wave-train. We shall suppose that  $f(x, y, z)$  is of the form :

$$f(x, y, z) = e^{-\frac{r^2}{2\sigma^2}} e^{-\frac{2\pi i}{h}(mv_x x + mv_y y + mv_z z)}, \quad (24)$$

where  $r^2$  is written for  $(x^2 + y^2 + z^2)$ .

The explanation of this particular choice of  $f$  will be clear from the following considerations. We suppose that at instants in the neighbourhood of  $t = 0$  the wave-train is of the form studied above (Chap. IV, § 3), viz. :

$$\psi(x, y, z, t) = A(x, y, z, t) e^{2\pi i \left( vt - \frac{\alpha x + \beta y + \gamma z}{\lambda} \right)}, \quad (25)$$

where  $\lambda = \frac{h}{mv}$ . Thus at the time  $t = 0$ , this wave-train is reduced to :

$$\psi(x, y, z, 0) = A(x, y, z, 0) e^{-\frac{2\pi i}{h}(mv_x x + mv_y y + mv_z z)}, \quad (26)$$

and the probability that at this instant the particle will be situated at the point  $(x, y, z)$  is  $A^2(x, y, z, 0)$ . Now we take the instant  $t = 0$  as the starting-point for the calculation, since it is supposed that an observation has been made upon the particle at that time. The result of this initial observation makes it possible for us to state that the most probable position of the particle after the observation is a certain point P which for simplicity we shall choose as the origin of co-ordinates. But there will be a certain possible error and by the Gaussian law of errors, the result of the observation must be stated thus : the probability that the particle is situated at the point  $(x, y, z)$  is  $e^{-\frac{r^2}{\sigma^2}}$ ,  $\sigma$  being the smaller the more accurately the experiment is made. As soon as the distance from the point  $(x, y, z)$  to the origin is a small multiple of  $\sigma$  the probability that the initial co-ordinates are  $(x, y, z)$  becomes very small ; we can thus say that the region in which the particle can be found at the initial instant has dimensions of the order of  $\sigma$ . According to the interference principle we have :

$$A^2(x, y, z, 0) = e^{-\frac{r^2}{\sigma^2}}; \quad A(x, y, z, 0) = e^{-\frac{r^2}{2\sigma^2}}, \quad (27)$$

and finally we are led to adopt the form proposed in (24) for  $f$ . The general form (23) becomes in this case :

$$\psi(x, y, z, t) = \left(\frac{im}{ht}\right)^{\frac{3}{2}} \prod_{xyz} \int_{-\infty}^{+\infty} e^{-\left\{\frac{x_0^2}{2\sigma^2} + \frac{2\pi im}{h} v_x x_0 + \frac{\pi im}{ht} (x - x_0)^2\right\}} dx_0, \quad (28)$$

where the symbol  $\prod_{xyz}$  denotes the product of the factor which follows it by those obtained by replacing  $x_0$  and  $x$ , by  $y_0$  and  $y$ , then by  $z_0$  and  $z$  respectively.

Writing :

$$a = \frac{1}{2\sigma^2} + \frac{\pi im}{ht}, \quad b_x = \frac{2\pi im}{ht}(x - v_x t), \quad (29)$$

the formula (28) may be written more simply :

$$\psi(x, y, z, t) = \left(\frac{im}{ht}\right)^{\frac{3}{2}} \prod_{xyz} e^{-\frac{\pi im}{ht} x^2} \int_{-\infty}^{+\infty} e^{-(ax_0^2 - b_x x_0)} dx_0. \quad (30)$$

But

$$\begin{aligned} \int_{-\infty}^{+\infty} e^{-(ax_0^2 - b_x x_0)} dx_0 &= e^{\frac{b_x^2}{4a}} \int_{-\infty}^{+\infty} e^{-a\left(x_0 - \frac{b_x}{2a}\right)^2} dx_0 \\ &= \frac{e^{\frac{b_x^2}{4a}}}{\sqrt{a}} \int_{-\infty}^{+\infty} e^{-z^2} dz = e^{\frac{b_x^2}{4a}} \sqrt{\frac{\pi}{a}}, \quad (31) \end{aligned}$$

and consequently

$$\psi(x, y, z, t) = \left(\frac{\pi im}{ah}\right)^{\frac{3}{2}} \prod_{xyz} e^{\left(\frac{b_x^2}{4a} - \frac{\pi im}{ht} x^2\right)}, \quad (32)$$

the factor  $\sqrt{\frac{\pi}{a}}$  occurring three times.

We have :

$$\left(\frac{\pi im}{ah}\right)^{\frac{3}{2}} = \frac{1}{\left(1 + \frac{ht}{2\pi im\sigma^2}\right)^{\frac{3}{2}}} = \left(\frac{\sigma}{\sqrt{\sigma^2 + \frac{ht}{2\pi im}}}\right)^3, \quad (33)$$

and

$$\frac{b_x^2}{4a} = \frac{\frac{\pi im}{ht}(x - v_x t)^2}{1 - \frac{iht}{2\pi m\sigma^2}}. \quad (34)$$

If we get rid of the imaginary in the denominator we obtain :

$$\frac{b_x^2}{4a} = \frac{\frac{\pi i m}{\hbar} \sigma^2 - \frac{1}{2}}{\sigma^2 + \left(\frac{\hbar t}{2\pi m \sigma}\right)^2} (x - v_x t)^2, \quad (35)$$

thus finally :

$$\psi(x, y, z, t) = \left( \frac{\sigma}{\sqrt{\sigma^2 + \left(\frac{\hbar t}{2\pi i m}\right)^2}} \right)^3 e^{-\frac{1}{2} \cdot \frac{(x - v_x t)^2 + (y - v_y t)^2 + (z - v_z t)^2}{\sigma^2 + \left(\frac{\hbar t}{2\pi m \sigma}\right)^2}} \\ e^{\frac{\pi i m}{\hbar} \cdot \frac{\sigma^2 \{(x - v_x t)^2 + (y - v_y t)^2 + (z - v_z t)^2\}}{\sigma^2 + \left(\frac{\hbar t}{2\pi m \sigma}\right)^2}} \times e^{-\frac{\pi i m}{\hbar} (x^2 + y^2 + z^2)}. \quad (36)$$

If we write as usual  $\psi = a e^{\frac{2\pi i \phi}{\hbar}}$ ,  $a$  and  $\phi$  being real quantities, we find :

$$a(x, y, z, t) = \sqrt{\psi \psi^*} \\ = \left\{ \frac{\sigma}{\sqrt{\sigma^2 + \left(\frac{\hbar t}{2\pi m \sigma}\right)^2}} \right\}^3 e^{-\frac{1}{2} \cdot \frac{(x - v_x t)^2 + (y - v_y t)^2 + (z - v_z t)^2}{\sigma^2 + \left(\frac{\hbar t}{2\pi m \sigma}\right)^2}}, \quad (37)$$

$$\phi(x, y, z, t) = \frac{m}{2t} \left[ \frac{\sigma^2}{\sigma^2 + \left(\frac{\hbar t}{2\pi m \sigma}\right)^2} \{(x - v_x t)^2 + (y - v_y t)^2 + (z - v_z t)^2\} - (x^2 + y^2 + z^2) \right] \\ + F(t), \quad (38)$$

where  $F(t)$  is a certain function of the time which we need not determine.

If we suppose that the dimensions of the wave-train are very large with respect to the wave-length  $\lambda = \frac{h}{mv}$ , then  $\sigma \gg \frac{h}{mv}$ . If we consider a value of  $t$  which is not very large compared with the reduced period  $\frac{h}{\frac{1}{2}mv^2}$ , we have :

$$\frac{h^2}{m^2 v^2} \sim \frac{\hbar t}{m},$$

where the symbol denotes that the two sides are of the same

order. Thus, since  $\sigma^2 \gg \frac{h^2}{m^2 v^2}$ , we can neglect  $\frac{ht}{2\pi m \sigma}$  in comparison with  $\sigma$ , and (36) is reduced to :

$$\psi(x, y, z, t) = e^{-\frac{(x-v_x t)^2 + (y-v_y t)^2 + (z-v_z t)^2}{2\sigma^2}} \cdot e^{\frac{2\pi i}{h} \{ \frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) t - m v_x x - m v_y y - m v_z z \}}. \quad (39)$$

The wave-train will have preserved the same form as it had at the beginning, the amplitude being carried forward in the direction of propagation with the velocity  $(v_x, v_y, v_z)$ . These are the conditions under which the approximate results of Chapter IV are valid. But here we see that they are valid for a limited time only. A time arrives in every case when the factor  $\frac{ht}{2\pi m \sigma}$  is no longer negligible compared with  $\sigma$  and the amplitude round the point with co-ordinates  $x = v_x t$ ,  $y = v_y t$ ,  $z = v_z t$ , is again expressed by a Gaussian function in which  $\sigma^2$  must be replaced by  $\sigma^2 + \left(\frac{ht}{2\pi m \sigma}\right)^2$ . There is a continuous spreading of the wave-train.

The same result may be obtained by considering the motion of the probability.

The velocity of the probability elements is equal to  $-\frac{1}{m} \text{grad } \phi$ ; its components are denoted by  $(\xi, \eta, \zeta)$  to avoid confusion with  $(v_x, v_y, v_z)$ , which are given constants. We have therefore by (38) :

$$\xi = -\frac{1}{m} \frac{\partial \phi}{\partial x} = v_x + \left(\frac{x}{t} - v_x\right) \frac{\left(\frac{ht}{2\pi m \sigma}\right)^2}{\sigma^2 + \left(\frac{ht}{2\pi m \sigma}\right)^2}. \quad (40)$$

together with similar equations for  $\eta$  and  $\zeta$ .

When  $t$  is sufficiently small, all the probability elements move approximately with the velocity  $\mathbf{v}$ ; the probability cloud moves as a whole in the direction of propagation with this velocity. But with increase of time the probability elements acquire a velocity component perpendicular to the direction of propagation which tends to extend the wave-train. At

the same time the probability elements situated in the forward part of the wave-train acquire in the direction of propagation a velocity greater than that of the elements situated behind, so that there is a progressive lengthening of the train. This is readily seen from the equations (40) by taking the  $z$ -axis as the direction of propagation and  $v_x = v_y = 0$ . The wave-train thus spreads slowly in all directions.

### 3. The Measurement of Velocity by Two Successive Observations

We retain the hypothesis (24) concerning the form of  $f(x, y, z)$  and consequently the expression (36) for  $\psi$ . The probability that an experiment made at time  $t$  will locate the particle in a volume element  $dx dy dz$  is therefore by (37) :

$$P(x, y, z, t) dx dy dz = a^2 dx dy dz. \quad . \quad . \quad (41)$$

We shall make use of this formula to discuss by means of a calculation the question of the determination of the velocity of the particle by two successive determinations of its position which was raised at the end of the last chapter.

We suppose that an initial observation made at zero time has made it possible to locate the particle at the origin of co-ordinates with a possible error of the order of  $\sigma$ . A second observation at time  $t$  attributes to the particle a position  $(x, y, z)$ , so that it is natural to say that the particle had the velocity  $u$  after the first observation with components given by :

$$u_x = \frac{x}{t}, \quad u_y = \frac{y}{t}, \quad u_z = \frac{z}{t}, \quad . \quad . \quad (42)$$

and that the momentum had the three components :

$$p_x = \frac{mx}{t}, \quad p_y = \frac{my}{t}, \quad p_z = \frac{mz}{t}. \quad . \quad . \quad (43)$$

It is true that these values are subject to an uncertainty of the order  $\frac{\sigma}{t}$  on account of the uncertainty about the exact initial position, but if there is a long interval between the two observations, it will be possible to make this uncertainty negligible. Since the wave-train in this case has time to

spread considerably between the two observations, the second observation might locate the particle in any point of an extended region of the space and the result is that in repeating the same observation under identical conditions, different values of  $x$ ,  $y$ ,  $z$ , and consequently of  $p_x$ ,  $p_y$ ,  $p_z$ , would be found. We cannot therefore say that  $p_x$ ,  $p_y$  and  $p_z$  have well-defined values and there are only certain probabilities for particular values.

We can construct a "momentum space" by means of the three variables ( $p_x$ ,  $p_y$ ,  $p_z$ ). Each determination of ( $x$ ,  $y$ ,  $z$ ) provides by (43) a point of this space, and to each element of volume  $dx dy dz$  corresponds by a well-known analytical theorem a volume  $dw$  of the momentum space given by :

$$\begin{aligned} dw &= \frac{\partial(p_x, p_y, p_z)}{\partial(x, y, z)} dx dy dz \\ &= \frac{m^3}{t^3} dx dy dz. \end{aligned} \quad (44)$$

The probability  $P(p_x, p_y, p_z, t)$  that an observation made at the time  $t$  will give a value of the components of momentum corresponding to a point in  $dw$  is equal to the probability of finding the particle in  $dx dy dz$ .

Thus :

$$P(p_x, p_y, p_z, t)dw = a^2(x, y, z, t) dx dy dz, \quad (45)$$

whence

$$P(p_x, p_y, p_z, t) = \frac{t^3}{m^3} a^2(x, y, z, t). \quad (46)$$

Since  $t$  is supposed very large, we may be content to write :

$$a^2(x, y, z, t) = \left( \frac{2\pi m \sigma^2}{ht} \right)^3 e^{-\frac{4\pi^2 m^2 \sigma^2}{h^2 t^2} \{ (x - v_x t)^2 + (y - v_y t)^2 + (z - v_z t)^2 \}}, \quad (47)$$

so that by (43) :

$$\frac{t^3}{m^3} a^2 = P = \left( \frac{2\pi \sigma^2}{h} \right)^3 e^{-\frac{4\pi^2 \sigma^2}{h^2} \{ (p_x - mv_x)^2 + (p_y - mv_y)^2 + (p_z - mv_z)^2 \}}. \quad (48)$$

The most probable values of  $p_x$ ,  $p_y$ ,  $p_z$  are thus  $mv_x$ ,  $mv_y$ ,  $mv_z$ , and if we denote the differences between the true and most probable values by  $\delta p_x$ ,  $\delta p_y$ ,  $\delta p_z$  and the uncertainties in

the initial co-ordinates by  $\delta x_0$ ,  $\delta y_0$ ,  $\delta z_0$  which are equal to  $\sigma$ , we have :

$$P(\delta p_x, \delta p_y, \delta p_z) = \left(\frac{2\pi\sigma^2}{h}\right)^3 e^{-4\pi^2\left\{\left(\frac{\delta x_0 \delta p_x}{h}\right)^2 + \left(\frac{\delta y_0 \delta p_y}{h}\right)^2 + \left(\frac{\delta z_0 \delta p_z}{h}\right)^2\right\}}. \quad (49)$$

It follows at once from (49) that the product of the uncertainty in the co-ordinates by that in the corresponding momenta after the first observation must be regarded as being of the order of magnitude of  $h$ . We arrive again at Heisenberg's conception.

#### 4. Rigorous Solution of the Propagation of a $\psi$ -Wave-train in a Uniform Constant Field of Force

The propagation of a wave-train in a uniform constant field of force is defined by the potential function :

$$F(x, y, z) = -(k_x x + k_y y + k_z z). \quad (50)$$

We shall in this case again try to find a transformation function. The wave-equation is :

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2}(k_x x + k_y y + k_z z)\psi = \frac{4\pi i m}{h} \frac{\partial \psi}{\partial t}, \quad (51)$$

and  $\psi(x, y, z, t)$  is completely determined if the initial value  $\psi(x, y, z, 0) = f(x, y, z)$  is given. The transformation function  $T(x, y, z, t, x_0, y_0, z_0)$  must be such that :

$$\psi(x, y, z, t) = \iiint f(x_0, y_0, z_0) T dx_0 dy_0 dz_0, \quad (52)$$

the limits of integration being  $-\infty$  to  $+\infty$ .

Thus  $T$  considered as a function of  $(x, y, z)$  must satisfy the equation :

$$\nabla^2 T + \frac{8\pi^2 m}{h^2}(k_x x + k_y y + k_z z)T = \frac{4\pi i m}{h} \frac{\partial T}{\partial t}. \quad (53)$$

As before, let us write :

$$T = R e^{\frac{2\pi i S}{h}}, \quad (54)$$

where  $R$  is a function of  $t$  and  $S$  of  $x, y, z, t, x_0, y_0, z_0$ .

We find on substituting (54) in (53) :

$$\frac{1}{2m} \sum \left( \frac{\partial S}{\partial x} \right)^2 + \sum k_x x = \frac{\partial S}{\partial t}, \quad . \quad . \quad (55)$$

$$m \frac{dR}{dt} = \frac{1}{2} R \nabla^2 S. \quad . \quad . \quad (56)$$

We can thus take for  $S$  Jacobi's function in the old mechanics which, as we have seen (Chap. II, § 6) is :

$$S = -\frac{m}{2t} \sum (x - x_0)^2 - \frac{1}{2} t \sum k_x (x + x_0) + \frac{t^3}{24m} \sum k_x^2, \quad (57)$$

and is a solution of equation (55). As in § 1 we find :

$$\nabla^2 S = -\frac{3m}{t}, \quad . \quad . \quad (58)$$

and by (56) :

$$R = Ct^{-\frac{3}{4}}. \quad . \quad . \quad (59)$$

It remains to verify that the function :

$$\psi = C \iiint_{t^{\frac{3}{2}}} e^{\frac{2\pi i}{h} S} dx_0 dy_0 dz_0 \quad . \quad . \quad (60)$$

reduces to  $f(x, y, z)$  at  $t = 0$ .

We again make the change of variables (15) and make use of (17) so that (60) becomes :

$$\psi = C \iiint f e^{\frac{2\pi i}{h} S} dr_1 dr_2 dr_3, \quad . \quad . \quad (61)$$

where in  $f$  and  $S$  it is supposed that  $x_0$ ,  $y_0$  and  $z_0$  have been replaced.

In the limit when  $t$  approaches zero it is found that :

$$\psi(x, y, z, 0) = C f(x, y, z) \int_{-\infty}^{+\infty} e^{-\frac{\pi i m}{h} r_1^2} dr_1 \int_{-\infty}^{+\infty} e^{-\frac{\pi i m}{h} r_2^2} dr_2 \int_{-\infty}^{+\infty} e^{-\frac{\pi i m}{h} r_3^2} dr_3, \quad (62)$$

and again it is only necessary to write  $C = \left( \frac{im}{h} \right)^{\frac{3}{2}}$  to obtain  $\psi(x, y, z, 0) = f(x, y, z)$ .



Finally, the expression :

$$\psi(x, y, z, t) = \left(\frac{im}{ht}\right)^{\frac{3}{2}} \iiint f e^{\frac{2\pi i}{h} S} dx_0 dy_0 dz_0 \quad . \quad (63)$$

is the solution of the wave-equation which assumes the value  $f(x, y, z)$  at  $t = 0$ , and is therefore the solution required.

### 5. Development of the Calculations in a Special Case

Let us adopt the form for  $f$  given by :

$$f = e^{-\frac{r^2}{2\sigma^2}} e^{-\frac{2\pi im}{h} \sum v_{0x} x}, \quad . \quad . \quad . \quad (64)$$

where  $r^2 = x^2 + y^2 + z^2$  and  $v_{0x}$ , etc., are the initial velocity components.

If we write  $S_x$  for that part of  $S$  which depends upon  $x$  and  $x_0$  we find :

$$\psi = \left(\frac{im}{ht}\right)^{\frac{3}{2}} \prod_{xyz} \int_{-\infty}^{\infty} e^{-\frac{x_0^2}{2\sigma^2} - \frac{2\pi im}{h} v_{0x} x_0} e^{\frac{2\pi i}{h} S_x} dx_0. \quad . \quad (65)$$

After making the substitutions :

$$a = \frac{1}{2\sigma^2} + \frac{\pi im}{ht}, \quad b_x = \frac{2\pi im}{ht} \left( x - v_{0x} t - \frac{k_x}{2m} t^2 \right), \quad . \quad (66)$$

(65) becomes :

$$\psi = \left(\frac{im}{ht}\right)^{\frac{3}{2}} \prod_{xyz} e^{-\frac{\pi im}{ht} x^2 - \frac{\pi i k_x t}{h} x + \frac{\pi i t^3 k_x^2}{12mh}} \int_{-\infty}^{\infty} e^{-ax_0^2 + b_x x_0} dx_0, \quad (67)$$

and the calculations made above give us in this case :

$$\psi = \left(\frac{\pi im}{hta}\right)^{\frac{3}{2}} \prod_{xyz} e^{\frac{b_x^2}{4a} - \frac{\pi im}{ht} x^2 - \frac{\pi i k_x t}{h} x + \frac{\pi i t^3 k_x^2}{12mh}}. \quad . \quad (68)$$

The value of  $\left(\frac{\pi im}{hta}\right)^{\frac{3}{2}}$  is that given in (33), and (35) is replaced by :

$$\frac{b_x^2}{4a} = \frac{\frac{\pi im}{ht} \sigma^2 - \frac{1}{2}}{\sigma^2 + \left(\frac{ht}{2\pi m \sigma}\right)^2} \left( x - v_{0x} t - \frac{1}{2} \frac{k_x}{m} t^2 \right)^2. \quad . \quad (69)$$

Thus the value of  $\psi$  is given by :

$$\psi = \left( \frac{\sigma}{\sqrt{\sigma^2 + \frac{ht}{2\pi m i}}} \right)^3 e^{-\frac{1}{2} \sum \frac{\left( x - v_0 x t - \frac{k_x x^2}{2m} \right)^2}{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2}} \\ \times e^{\frac{\pi i m}{ht} \left\{ \frac{\sigma^2 \sum \left( x - v_0 x t - \frac{k_x x^2}{2m} \right)^2}{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2} - \sum \left( x^2 + \frac{k_x x t^2}{m} - \frac{k_x^2 t^4}{12 m^2} \right) \right\}}. \quad (70)$$

According to the interference principle, the probability that the particle is situated at  $(x, y, z)$  at time  $t$  is :

$$a^2 = \psi \psi^* = \left( \frac{\sigma}{\sqrt{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2}} \right)^3 e^{-\frac{\sum \left( x - v_0 x t - \frac{k_x x^2}{2m} \right)^2}{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2}}, \quad (71)$$

and when it is permissible to neglect  $\left( \frac{ht}{2\pi m \sigma} \right)^2$  in comparison with  $\sigma^2$ , which would always be possible if  $h$  were infinitesimal, we have :

$$a^2 = e^{-\sum \left( x - v_0 x t - \frac{k_x x^2}{2m} \right)^2}. \quad (72)$$

In this case the wave-train has the same form about the point with co-ordinates :

$$x = v_0 x t - \frac{k_x}{2m} t^2, \quad y = v_0 y t - \frac{k_y}{2m} t^2, \quad z = v_0 z t - \frac{k_z}{2m} t^2,$$

at time  $t$  as it had about the origin at zero time. The wave-train moves as a whole and has throughout the same motion as in the classical theory, but when the term  $\left( \frac{ht}{2\pi m \sigma} \right)^2$  can be no longer neglected the dimensions of the wave-train increase, since  $\sigma$  is replaced by  $\sigma^1 = \sqrt{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2}$  and there is continuous spreading.

We arrive at the same conclusion by calculating the velocity of the probability elements. Let  $(\xi, \eta, \zeta)$  again denote the

components of this velocity. The expression (70) shows that the phase is given by :

$$\phi = \frac{m}{2t} \left\{ \frac{\sigma^2}{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2} \sum (x - v_{0x} t - \frac{k_x}{2m} t^2)^2 - \sum \left( x^2 + \frac{k_x}{m} x t^2 - \frac{k_x^2}{12m^2} t^4 \right) \right\} \quad (73)$$

omitting the additional term of the form  $F(t)$  which contributes nothing to  $(\xi, \eta, \zeta)$ .

From (73) we deduce :

$$\xi = -\frac{1}{m} \frac{\partial \phi}{\partial x} = v_{0x} + \frac{k_x}{m} t + \frac{\left( \frac{ht}{2\pi m \sigma} \right)^2}{\sigma^2 + \left( \frac{ht}{2\pi m \sigma} \right)^2} \left( \frac{x}{t} - v_{0x} - \frac{k_x}{2m} t \right) \quad (74)$$

together with similar expressions for  $\eta$  and  $\zeta$ .

These expressions show that if  $\left( \frac{ht}{2\pi m \sigma} \right)^2$  is negligible as before, the probability elements move as a whole with the velocity anticipated for the particles by the classical theory. But the situation changes when the term is appreciable and in addition to these classical velocities there appear centrifugal velocity components with respect to the point :

$$x = v_{0x} t + \frac{k_x}{2m} t^2, \quad y = v_{0y} t + \frac{k_y}{2m} t^2, \quad z = v_{0z} t + \frac{k_z}{2m} t^2,$$

and the wave-train tends to spread in all directions.

Let it be supposed that the velocity of the particle is determined by two observations made at zero time and at time  $t$  and let the second observation locate the particle at the point  $(x, y, z)$ . We can consider the initial velocity components as equal to :

$$U_{0x} = \frac{x}{t} - \frac{k_x}{2m} t, \quad U_{0y} = \frac{y}{t} - \frac{k_y}{2m} t, \quad U_{0z} = \frac{z}{t} - \frac{k_z}{2m} t. \quad (75)$$

The possible error due to the uncertainty  $\sigma$  in the original position can be diminished as much as we please by taking for  $t$  a sufficiently large value. By the argument of the preceding

paragraph we again find that the probability that a second observation will give values  $(p_{0x}, p_{0y}, p_{0z})$  for the original components of momentum is given by :

$$P(p_{0x}, p_{0y}, p_{0z}) = \left(\frac{2\pi\sigma^2}{h}\right)^3 e^{-\frac{4\pi^2\sigma^2}{h^2}\sum(p_{0x} - mv_{0x})^2} \quad . \quad (76)$$

The most probable values for  $p_{0x}$ ,  $p_{0y}$  and  $p_{0z}$  are therefore  $mv_{0x}$ ,  $mv_{0y}$  and  $mv_{0z}$ . Let us denote by  $\delta p_{0x}$ ,  $\delta p_{0y}$  and  $\delta p_{0z}$  the deviations between the true and most probable values, and let  $\delta x_0$ ,  $\delta y_0$  and  $\delta z_0$  be the uncertainties, which are equal to  $\sigma$ , in the initial co-ordinates, so that :

$$P(\delta p_{0x}, \delta p_{0y}, \delta p_{0z}) = \left(\frac{2\pi\sigma^2}{h}\right)^3 e^{-4\pi^2\sum\left(\frac{\delta p_{0x}\delta x_0}{h}\right)^2} \quad . \quad (77)$$

We have once more the Heisenberg relations between the uncertainties in the co-ordinates and in the conjugate momenta in the initial state after the first observation.

## CHAPTER XIV

### WAVE MECHANICS OF SYSTEMS OF PARTICLES

#### 1. Summary of the Principles of the Old Dynamics of Systems

**H**ITHERTO we have been occupied only with the case of a single particle moving in a given field of force.

But we have often to consider the case of an assembly of particles acting upon one another. We cannot then consider the field as given, since, if attention is paid to one of the particles of the system, that particular particle is subject to forces generated by the others, and these possess a motion dependent upon the particle itself. Thus it is necessary to determine at one and the same time the motion of all the particles, and this determination is the solution of the rather complicated problem which constitutes the subject of what is known as the dynamics of systems. We shall recall the principles of this, limiting ourselves to Newtonian mechanics.

In classical mechanics we pass very simply from the dynamics of a single material point to the dynamics of systems by admitting the principle of the equality of action and reaction, according to which the force exerted by a particle A on a particle B is equal and opposite to that exerted by B on A.

Let us consider a system of  $N$  particles numbered from 1 to  $N$  to which co-ordinates  $(x_i, y_i, z_i)$  are assigned, where  $i$  may have any value from 1 to  $N$ .

The Lagrangian function for the  $i$ th particle is :

$$L_i(x_i, y_i, z_i, \dot{x}_i, \dot{y}_i, \dot{z}_i, t) = T_i - F_i(x_1 \dots x_N, t), \quad (1)$$

$T_i$  being the kinetic energy  $\frac{1}{2}m_i(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2)$  of the particle.

$F_i$  is the potential energy of the  $i$ th particle depending upon the position of all the particles of the system and on the

external field of force to which the assembly may be subject. We will write it in the form :

$$F_i = \sum_j F_{ij} + f_i, \quad (j = 1 \text{ to } N), \quad . \quad . \quad . \quad (2)$$

where  $F_{ij}$  denotes that part of the potential energy of the  $i$ th particle which arises from the action of the  $j$ th particle upon it,  $F_{ii}$  being zero, since the particle is not considered to act upon itself.  $f_i$  denotes the action of the external field on the  $i$ th particle.

The principle of equality of action and reaction is expressed by the formula :

$$F_{ij} = F_{ji}^1. \quad . \quad . \quad . \quad . \quad (3)$$

In other words, the quantities  $F_{ij}$  form a symmetrical table with diagonal terms zero.

We can write down the Lagrangian equations for each particle as follows :

$$\frac{d}{dt} \left( \frac{\partial L_i}{\partial \dot{x}_i} \right) = \frac{\partial L_i}{\partial x_i} \quad . \quad . \quad . \quad . \quad (4)$$

with similar equations in  $y_i$  and  $z_i$ , and there are  $3N$  equations of this type in the assembly.

The classical dynamics of systems condenses these  $3N$  equations by introducing a Lagrangian function  $L$  defined by :

$$\begin{aligned} L(x_1, y_1, \dots, z_N, \dot{x}_1, \dot{y}_1, \dots, \dot{z}_N, t) &= \sum T_i - \frac{1}{2} \sum F_{ij} - \sum f_i \\ &= T - F, \quad . \quad . \quad . \quad (5) \end{aligned}$$

where  $\sum F_{ij}$  denotes a double summation over  $i$  and  $j$  and  $T = \sum T_i$ ,  $F = \frac{1}{2} \sum F_{ij} + f_i$ .

$L$  is the Lagrangian function for the whole system, and is not the sum of the individual Lagrangian functions, since it contains each term of mutual action once only. In the same way  $F$  is called the potential energy of the whole system ; it is

<sup>1</sup>  $F_{ij}$  and  $F_{ji}$  are, in fact, functions of  $r_{ij}$  alone, where  $r_{ij}$   
 $= \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$

is the distance between the  $i$ th and  $j$ th particles and the assumption of (3) implies that  $\frac{\partial F_{ij}}{\partial x_i} = - \frac{\partial F_{ji}}{\partial x_j}$  or the principle of action and reaction is satisfied.

not the sum of the potential energies of the various particles. By means of  $L$  the  $3N$  Lagrangian equations become :

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = \frac{\partial L}{\partial x_i}, \quad (i = 1 \text{ to } N) \quad . \quad . \quad . \quad (6)$$

with the corresponding equations in  $y$  and  $z$ .

As we have now Lagrangian equations with a single function  $L$  depending upon all the co-ordinates of the particles of the system, we shall be able to find a principle of stationary action for the whole system. Consider therefore a space of  $3N + 1$  dimensions built up by the  $3N$  co-ordinates and the time. The motion of the whole system is represented by a line in this space, each point of the line corresponding to an arrangement of the system at a particular time. The line representing the motion between two points  $P$  and  $Q$  from time  $t_0$  to time  $t_1$  is defined by the Hamiltonian principle that the integral :

$$\int_{t_0}^{t_1} L dt \quad . \quad . \quad . \quad . \quad . \quad (7)$$

taken along it is stationary for all infinitely small displacements from it with the extremities fixed. This principle is valid, since it takes us by the classical procedure of the calculus of variations to the  $3N$  Lagrangian equations (6). Moreover, this Hamiltonian principle has an intrinsic significance independent of the choice of variables assigned to the system. Thus, if the  $3N$  co-ordinates  $(x_i, y_i, z_i)$  are expressible in terms of  $n$  variables,  $q_k$ , in the form :

$$x_i = f_i(q_1 \dots q_n), \quad y_i = \phi_i(q_1 \dots q_n), \quad z_i = \psi_i(q_1 \dots q_n), \quad (8)$$

the function  $L$  will be expressible in terms of the  $(2n + 1)$  variables  $q_k, \dot{q}_k$  and  $t$ . We shall have therefore :

$$\delta \int_{t_0}^{t_1} L(q_k, \dot{q}_k, t) dt = 0 \quad . \quad . \quad . \quad . \quad (9)$$

the limits  $t_0$  and  $t_1$  not being subject to variation. In general  $n$  is equal to  $3N$ , but if there are any constraints, that is to say, if certain relations<sup>1</sup> exist between the co-ordinates of the  $N$  particles,  $n$  may be less than  $3N$ . The number of independent

<sup>1</sup> We suppose, for the sake of simplicity, that the constraints are independent of the time.

variables which are necessary to define the system is called the number of degrees of freedom.

As in the case of the single material point we define certain momenta  $p_i$  conjugate to the co-ordinates  $q_i$  by the relations :

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \quad (i = 1 \text{ to } n), \quad . \quad . \quad . \quad (10)$$

which makes it possible to write the Lagrangian equations in the form :

$$\frac{dp_i}{dt} = \frac{\partial L}{\partial q_i}, \quad (i = 1 \text{ to } n). \quad . \quad . \quad . \quad (11)$$

In the same way we shall describe as the energy the quantity :

$$W = \sum p_i \dot{q}_i - L \quad . \quad . \quad . \quad (12)$$

and since by (10) and (11) we have :

$$\begin{aligned} \frac{dW}{dt} &= \sum \frac{dp_i}{dt} \dot{q}_i + \sum p_i \frac{d\dot{q}_i}{dt} - \sum \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i - \sum \frac{\partial L}{\partial \dot{q}_i} \frac{d\dot{q}_i}{dt} - \frac{\partial L}{\partial t} \\ &= -\frac{\partial L}{\partial t}, \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (13) \end{aligned}$$

we conclude that if the external field is independent of the time, or  $\frac{\partial L}{\partial t} = 0$ , the quantity  $W$  remains constant.

By the definition (12) of  $W$  we can express the Hamiltonian integral as a line integral in the space of  $(n + 1)$  dimensions formed by the  $n$  co-ordinates  $q_i$  and the time, for we have :

$$\int_{t_0}^{t_1} L dt = \int_P^Q (\sum p_i dq_i - W dt), \quad . \quad . \quad . \quad (14)$$

$P$  and  $Q$  being the extremities of the line representing the path of the motion in the  $q$ - $t$  space.

In the case in which the external field of force does not depend on the time, and where in consequence the energy remains constant, the Hamiltonian principle leads to the principle of least action of Maupertuis. Let us consider a generalised space formed by the  $q$  co-ordinates alone ; this space will play an important part in what follows. The assembly of positions of the particles of the system at a given instant is denoted by a representative point in this space, and



the motion of the particles of the system is represented by a curve or trajectory of the representative point in the generalised space. The principle of least action of Maupertuis may be described by the statement that the trajectory of the representative point between two points A and B of the generalised space is such that the line integral  $\int_A^B \sum p_i dq_i$  taken along the trajectory is stationary for any infinitely small variation which leaves unaltered the limits A and B and the energy W. The proof by Hamilton's principle is exactly the same as that of Chapter I, § 4, except for the circumstance that there are now  $n$  variables instead of 3.

Similarly, by resuming the proofs of Chapter I, §§ 5-6, by merely changing  $\sum_1^3$  to  $\sum_1^n$  we shall find first the Hamiltonian equations :

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad (i = 1 \dots n) \quad (15)$$

then the theorem of contact transformations which is now expressed in the statement that the transformations  $\alpha_i = f_i(q_k, p_k, t)$  and  $\beta_i = \phi_i(q_k, p_k, t)$ , subject to the condition,

$$\sum_1^n p_i dq_i - \sum_1^n \beta_i d\alpha_i = -[dS]_t, \quad (16)$$

maintain the canonical form of the Hamilton equations if  $H$  is replaced by  $K = H - \frac{\partial S}{\partial t}$ , expressed in the new variables.

Here, as in the earlier chapter, the notation means that the differential of  $S$  is made without varying  $t$ .

By means of this theorem we can develop as before the theory of Jacobi's equation (Chap. II) and arrive at Jacobi's theorem that if it is possible to obtain a complete integral, i.e. one depending upon  $n$  arbitrary constants  $\alpha_i$ , of the first order partial differential equation :

$$H\left(q_i, -\frac{\partial S}{\partial q_i}, t\right) = \frac{\partial S}{\partial t} \quad (17)$$

we shall have :

$$p_i = -\frac{\partial S}{\partial q_i}, \quad \beta_i = \frac{\partial S}{\partial \alpha_i}, \quad (i = 1 \dots n) \quad (18)$$

where  $S$  depends upon  $q_i$ ,  $\alpha_i$  and  $t$  and the  $\beta$ 's are  $n$  new constants. The equations (18), which define the  $2n$  quantities  $q_i$  and  $p_i$  as functions of the time and the  $2n$  constants  $\alpha_i$  and  $\beta_i$ , give completely the motion of the system of  $n$  degrees of freedom.

## 2. Transition from the Old to the New Dynamics of Systems

To pass from the wave mechanics of a single particle to the wave mechanics of systems of particles, we cannot proceed as in the old mechanics. If we wished to follow this route it would be necessary to consider the motion of each particle and its associated wave under the action of the fields created by the other particles and of the external field, if it exists. Then by introducing the principle of action and reaction it would be necessary to solve simultaneously the problem of the propagation of the  $N$  waves associated with the  $N$  particles of the system. It appears hardly possible to proceed in this way, the chief reason being the difficulty of locating each particle at a point in its wave; we cannot express the field of force acting upon a particle in terms of the positions of the others, since these positions are not well defined. In order to construct the wave mechanics of systems Schrödinger has followed a quite different path which, while raising certain difficulties of principle, has given very good results and with which we have at present to be content. But he has in his attempt succeeded in obtaining only the non-relativistic equations; the relativistic wave mechanics of systems is still lacking.

Schrödinger assumes the existence of the generalised space of  $n$  dimensions formed by the variables  $q_1 \dots q_n$ , which define the system of  $n$  degrees of freedom to be considered.

He associates with the motion of the system not as many waves travelling in ordinary space as there are particles, but a single wave travelling in the generalised space. He has sought an equation for this wave which, to the approximation of geometrical optics, is in harmony with the old mechanics. Following Schrödinger's idea we must therefore seek a wave equation depending upon the variables  $q_1, \dots, q_n, t$ , such that, if the solution be written in the form :

$$\psi = ae^{\frac{2\pi i}{h} \phi}, \quad . \quad . \quad . \quad (19)$$

where  $\psi$ ,  $a$  and  $\phi$  depend upon the variables and the time, the conditions are realised (1) that when the approximations of geometrical optics are realised, in particular, when  $h$  is considered infinitely small, the function  $\phi$  will coincide with Jacobi's function of the old mechanics, (2) that if the system consists of a single particle we must obtain the wave equation for a single particle, and (3) if the system consists of  $N$  particles which do not interact, the wave equation must split up into  $N$  separate equations of the type valid for a single particle.

But before studying a propagation in generalised space we must complete the definition of it by attributing to it a metric in the Riemannian sense, that is to say, we must assume that the square of the element of length corresponding to a variation of the co-ordinates  $q_i$  of amount  $dq_i$  is given at each point by the quadratic expression  $ds^2 = \sum_{ik} g_{ik} dq_i dq_k$ , where as usual summation over the possible values of  $i$  and  $k$  is implied. We shall see how the  $g_{ik}$  must be chosen, but must first recall certain mathematical formulæ which we require.

### 3. Mathematical Results

Let us consider a space of  $n$  dimensions and suppose, in the first place, that the points have  $n$  co-ordinates  $(x_1, \dots, x_n)$  such that the surfaces,  $x_i = \text{constant}$ , cut one another at right angles, which simply means that we have chosen a system of orthogonal co-ordinates. In the neighbourhood of each point it is as if we had chosen a rectangular Cartesian system of co-ordinates and the square of the element of length takes the form :

$$ds^2 = \sum dx_i^2. \quad . \quad . \quad . \quad (20)$$

The element of volume will be :

$$d\tau = dx_1 dx_2 \dots dx_n. \quad . \quad . \quad . \quad (21)$$

By means of a transformation of the variables :

$$q_i = f_i(x_1 \dots x_n),$$

we then define any  $n$  curvilinear co-ordinates. Conversely, the  $x_i$  may be considered as functions of the  $q_i$  and the expression for  $dx_i^2$  may be written :

$$dx_i^2 = \sum_{jk} \frac{\partial x_i}{\partial q_j} \frac{\partial x_i}{\partial q_k} dq_j dq_k. \quad . \quad . \quad . \quad (22)$$

and in consequence we have :

$$ds^2 = \sum_{ijk} \frac{\partial x_i}{\partial q_j} \frac{\partial x_i}{\partial q_k} dq_j dq_k = \sum g_{jk} dq_j dq_k, \quad (23)$$

where

$$g_{jk} = \sum_i \frac{\partial x_i}{\partial q_j} \frac{\partial x_i}{\partial q_k}, \quad (24)$$

and evidently

$$g_{jk} = g_{kj}. \quad (25)$$

Let  $\left| \frac{\partial x_i}{\partial q_j} \right|$  denote the determinant with the general term  $\frac{\partial x_i}{\partial q_j}$ ; it is the Jacobian  $\frac{\partial(x_1, \dots, x_n)}{\partial(q_1, \dots, q_n)}$  of the  $x$ 's with respect to the  $q$ 's. By the multiplication rule of determinants :

$$\left| \frac{\partial x_k}{\partial q_i} \right|^2 = \left| \sum_j \frac{\partial x_j}{\partial q_i} \frac{\partial x_j}{\partial q_k} \right| = |g_{ik}|, \quad (26)$$

so that if  $g$  denotes the determinant of the terms  $g_{ik}$ , we have :

$$g = \left\{ \frac{\partial(x_1, \dots, x_n)}{\partial(q_1, \dots, q_n)} \right\}^2. \quad (27)$$

The well-known analytical theorem for change of variables then gives :

$$d\tau = dx_1 \dots dx_n = \sqrt{g} dq_1 \dots dq_n, \quad (28)$$

and in this way we obtain the element of volume in terms of the  $q_i$ 's and  $g_{ik}$ 's.

$\gamma_{ik}$  being the minor of  $g_{ik}$  in the determinant  $g$ , we write :

$$g^{ik} = \frac{\gamma_{ik}}{g}, \quad (29)$$

whence  $g^{ik} = g^{ki}$  and by the properties of determinants :

$$\sum_k g^{ik} g_{kl} = 1 \text{ or } 0 \quad (30)$$

according as  $i = l$  or  $i \neq l$ .

This formula represents  $n^2$  linear equations which completely determine the  $n^2$  quantities  $g^{ik}$  as functions of the  $g_{ik}$ , and we can readily verify that :

$$g^{kl} = \sum_j \frac{\partial q_k}{\partial x_j} \frac{\partial q_l}{\partial x_j}. \quad (31)$$

We have by (24) :

$$\begin{aligned}\sum_k g^{ik} g_{kl} &= \sum_k \left( \sum_j \frac{\partial q_i}{\partial x_j} \frac{\partial q_k}{\partial x_j} \sum_m \frac{\partial x_m}{\partial q_k} \frac{\partial x_m}{\partial q_l} \right) \\ &= \sum_{jm} \frac{\partial q_i}{\partial x_j} \frac{\partial x_m}{\partial q_j} \sum_k \frac{\partial q_k}{\partial x_j} \frac{\partial x_m}{\partial q_k}, \quad . \quad . \quad (32)\end{aligned}$$

and the product under  $\sum_k$  vanishes unless  $j = m$ , when it is equal to unity. We have, therefore :

$$\sum_k g^{ik} g_{kl} = \sum_j \frac{\partial q_i}{\partial x_j} \frac{\partial x_j}{\partial q_l} = \frac{\partial q_i}{\partial q_l}, \quad . \quad . \quad (33)$$

which vanishes unless  $i = l$  and is then equal to unity. The equations (30) are thus satisfied by (31).

We pass on finally to determine the general expression for the Laplacian operator in terms of general co-ordinates,  $q_i$ , the operation on a function  $f$  being by definition  $\sum_i \frac{\partial^2 f}{\partial x_i^2}$ . We will

begin with the statement that if  $f$  is a function of the  $n$  co-ordinates, which is finite, uniform and continuous throughout the  $n$ -dimensional space considered and which is zero at infinity, the equation :

$$\sum_i \frac{\partial^2 f}{\partial x_i^2} = 0 \quad . \quad . \quad . \quad (34)$$

is the expression of the fact that the integral  $\int \sum_i \left( \frac{\partial f}{\partial x_i} \right)^2 d\tau$

extended throughout all space is stationary for any infinitely small variation in the form of  $f$  which does not violate the continuity and uniformity of this function. The integral and the space are, of course,  $n$ -dimensional and  $d\tau$  is an element of volume  $dx_1 dx_2 \dots dx_n$ . If  $f$  varies by  $\delta f$  at each point of this space the above integral undergoes the change :

$$\delta \int \sum_i \left( \frac{\partial f}{\partial x_i} \right)^2 d\tau = \int 2 \sum_i \frac{\partial f}{\partial x_i} \delta \left( \frac{\partial f}{\partial x_i} \right) d\tau = - \int 2 \sum_i \frac{\partial^2 f}{\partial x_i^2} \delta f d\tau, \quad (35)$$

and in order that this change may be zero whatever the value of  $\delta f$ , it is both necessary and sufficient that equation (34) be true.

We can also express the integral to be varied in terms of the  $q$  co-ordinates by a change of variables from  $x$  to  $q$ . We have :

$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i}, \quad \left( \frac{\partial f}{\partial x_i} \right)^2 = \sum_{k,l} \frac{\partial f}{\partial q_k} \frac{\partial f}{\partial q_l} \frac{\partial q_k}{\partial x_i} \frac{\partial q_l}{\partial x_i}, \quad (36)$$

and

$$\sum_i \left( \frac{\partial f}{\partial x_i} \right)^2 = \sum_{kl} \frac{\partial f}{\partial q_k} \frac{\partial f}{\partial q_l} \sum_i \frac{\partial q_k}{\partial x_i} \frac{\partial q_l}{\partial x_i} = \sum_{kl} g^{kl} \frac{\partial f}{\partial q_k} \frac{\partial f}{\partial q_l} \quad (37)$$

by (31). From this we deduce :

$$\begin{aligned} \delta \int \sum_i \left( \frac{\partial f}{\partial x_i} \right)^2 d\tau &= \delta \int \sum_{k,l} g^{kl} \frac{\partial f}{\partial q_k} \frac{\partial f}{\partial q_l} \sqrt{g} dq_1 \dots dq_n \\ &= \int 2 \sum_{k,l} g^{kl} \frac{\partial f}{\partial q_k} \delta \left( \frac{\partial f}{\partial q_l} \right) \sqrt{g} dq_1 \dots dq_n \\ &= - \int 2 \sum_{k,l} \frac{\partial}{\partial q_l} \left( \sqrt{g} g^{kl} \frac{\partial f}{\partial q_k} \right) \delta f dq_1 \dots dq_n. \quad (38) \end{aligned}$$

If we compare this with (35), the latter being another expression of the same quantity, remembering that :

$$d\tau = \sqrt{g} dq_1 \dots dq_n, \quad (39)$$

we see that :

$$\sum_i \frac{\partial^2 f}{\partial x_i^2} = \frac{1}{\sqrt{g}} \sum_{kl} \frac{\partial}{\partial q_l} \left( \sqrt{g} g^{kl} \frac{\partial f}{\partial q_k} \right). \quad (40)$$

This is the generalised expression of the Laplace operation in  $n$  dimensions in any co-ordinates,  $q$ . Of course, if  $n = 3$ , we have the ordinary operation in curvilinear co-ordinates.

#### 4. The Wave Equation in Generalised Space

A metric must be associated with the space before we can consider propagation in it, and for this purpose we begin with the kinetic energy of the system, and since Schrödinger's wave mechanics is non-relativistic we shall begin with the expression :

$$T = \sum_i \frac{1}{2} m_i (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) \quad (41)$$

for the kinetic energy, where  $(x_i, y_i, z_i)$  denote the rectangular co-ordinates of the  $i$ th particle,  $m_i$  its mass and the number of particles is  $N$ . If the system has  $n$  degrees of freedom, the  $3N$  co-ordinates may be expressed by  $n$  co-ordinates  $q_1 \dots q_n$ . The velocities are expressible linearly in the  $\dot{q}$ 's and  $T$  becomes a homogeneous quadratic in these quantities, since it is assumed that  $t$  does not occur explicitly in the relations between the  $x$ 's and the  $q$ 's :

$$T = \frac{1}{2} \sum_{i,k} \mu_{ik} \dot{q}_i \dot{q}_k, \quad . \quad . \quad . \quad (42)$$

where the quantities  $\mu_{ik}$  are in general functions of the  $q$ 's and  $\mu_{ik} = \mu_{ki}$ .

The Lagrangian function,  $L = T - F$ , depends upon the  $q$ 's through  $T$  only, so that :

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i} = \sum_k \mu_{ik} \dot{q}_k, \quad (i = 1, 2, \dots n). \quad (43)$$

This equation represents a system of  $n$  linear equations expressing the  $p$ 's in terms of the  $\dot{q}$ 's and they can in general be solved to give the  $\dot{q}$ 's in terms of the  $p$ 's. Let  $\nu_{ik}$  denote the minor of  $\mu_{ik}$  in the determinant  $|\mu_{ik}| = \mu$  and write :

$$\mu^{ik} = \frac{\nu^{ik}}{\mu}, \quad . \quad . \quad . \quad (44)$$

so that we find :

$$\dot{q}_i = \sum_k \mu^{ik} p_k, \quad (i = 1, 2, \dots n). \quad (45)$$

We may easily find the classical form of Jacobi's equation. The energy expressed as a function of the  $q$ 's,  $p$ 's and the time is :

$$H(q_i, p_i, t) = \sum \frac{1}{2} \mu_{ik} \mu^{ij} p_j \mu^{kl} p_l + F(q_i, t), \quad . \quad (46)$$

where the summation applies to all the suffixes and  $F$  is the potential energy of the system.

By the theory of determinants :

$$\sum_k \mu_{ik} \mu^{kl} = 1 \text{ or } 0 \quad . \quad . \quad . \quad (47)$$

according as  $i = l$  or  $i \neq l$ , and therefore :

$$H(q_i, p_i, t) = \frac{1}{2} \sum_{ij} \mu^{ij} p_i p_j + F(q_i, t) \quad . \quad . \quad (48)$$

and (17) may be written :

$$\frac{1}{2} \sum_{ij} \mu^{ij} \frac{\partial S}{\partial q_i} \frac{\partial S}{\partial q_j} + F(q_i, t) = \frac{\partial S}{\partial t}. \quad (49)$$

The metric of this space will be defined by making  $\mu_{ik}$ ,  $\mu^{ik}$  and  $\mu$  play the part of  $g_{ik}$ ,  $g^{ik}$  and  $g$  in the last paragraph, or we define the expression  $ds^2$  by the formula :

$$ds^2 = \sum_{ik} \mu_{ik} dq_i dq_k. \quad (50)$$

The element of volume is then :

$$d\tau = \sqrt{\mu} dq_1 \dots dq_n \quad (51)$$

and the generalised Laplacian operator :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial}{\partial q_k} \right). \quad (52)$$

We have assumed that the non-relativistic equation for a single particle of mass  $m$  which the wave function satisfies is :

$$\frac{1}{m} \nabla^2 \psi - \frac{8\pi^2}{h^2} F\psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t}. \quad (53)$$

Schrödinger has transposed this expression and adopted as the wave equation in the generalised space :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial \psi}{\partial q_k} \right) - \frac{8\pi^2}{h^2} F(q_i, t) \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} \quad (54)$$

We must make sure that this expression satisfies the three conditions stated in § 2 of this chapter.

1. When the conditions of geometrical optics are satisfied and in particular when  $h$  can be considered infinitely small, the function  $\phi$  satisfies Jacobi's equation.

Let us write as usual  $\psi = ae^{\frac{2\pi i}{h} \phi}$  where the variables are the  $q$ 's and  $t$  and  $a$  and  $\phi$  are real. Substituting in (54) and equating to zero the real terms, then neglecting in the equation thus obtained the terms which do not contain  $h^2$  in the denominator, we find :

$$\frac{1}{2} \sum_{ij} \mu^{ij} \frac{\partial \phi}{\partial q_i} \frac{\partial \phi}{\partial q_j} + F(q_i, t) = \frac{\partial \phi}{\partial t}. \quad (55)$$



The function  $\phi$  thus satisfies Jacobi's equation (49) and to this degree of approximation it may be regarded as the Jacobian function of the old mechanics.

2. If the system consists of a single particle we obtain once more equation (53).

Let us denote the mass of the particle by  $m$  and take rectangular axes of co-ordinates. We have  $T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$ , and therefore in this case :

$$\mu_{ik} = \begin{cases} m & \text{for } i = k \\ 0 & \text{for } i \neq k \end{cases}, \quad \mu = m^3, \quad \mu^{ik} = \begin{cases} \frac{1}{m} & \text{for } i = k \\ 0 & \text{for } i \neq k \end{cases}, \quad \begin{cases} i \\ k \end{cases} = 1, 2, 3. \quad (56)$$

The equation (54) when applied to this special case becomes (53).

3. If the system is formed by  $N$  particles which do not react upon one another the wave equation splits up into  $N$  separate equations of the type valid for a single particle.

Let  $m_i$  denote the mass of the  $i$ th particle, and let the co-ordinates be chosen rectangular.

We have :

$$T = \sum_i \frac{1}{2} m_i (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2),$$

and in this case :

$$\left. \begin{aligned} \mu_{ik} &= 0 \text{ for } i \neq k, \quad \mu_{11} = \mu_{22} = \mu_{33} = m_1 \text{ and in general} \\ \mu_{3i-2, 3i-2} &= \mu_{3i-1, 3i-1} = \mu_{3i, 3i} = m_i, \quad \mu = m_1^3 m_2^3 \dots m_N^3 \\ \mu^{ik} &= 0 \text{ for } i \neq k, \quad \mu^{11} = \mu^{22} = \mu^{33} = \frac{1}{m_1} \text{ and in general} \\ \mu^{3i-2, 3i-2} &= \mu^{3i-1, 3i-1} = \mu^{3i, 3i} = \frac{1}{m_i} \end{aligned} \right\} \quad (57)$$

$F$  in this case becomes  $\sum_i F_i(x_i, y_i, z_i, t)$ , and equation (54) is reduced to the form :

$$\sum_i \left\{ \frac{1}{m_i} \left( \frac{\partial^2 \psi}{\partial x_i^2} + \frac{\partial^2 \psi}{\partial y_i^2} + \frac{\partial^2 \psi}{\partial z_i^2} \right) - \frac{8\pi^2}{h^2} F_i \psi \right\} = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} \quad (58)$$

If we write  $\psi$  in the form :

$$\psi = \psi_1 \psi_2 \dots \psi_N, \quad . \quad . \quad . \quad (59)$$

where  $\psi$  is a function of all the variables while  $\psi_i$  is a function of  $x_i, y_i, z_i$  and  $t$  only, we obtain  $N$  equations of the form :

$$\begin{aligned} \frac{1}{m_i} \left( \frac{\partial^2 \psi_i}{\partial x_i^2} + \frac{\partial^2 \psi_i}{\partial y_i^2} + \frac{\partial^2 \psi_i}{\partial z_i^2} \right) - \frac{8\pi^2}{h^2} F_i \psi_i \\ = \frac{4\pi i}{h} \frac{\partial \psi_i}{\partial t} \quad (i = 1, 2, \dots, N) \end{aligned} \quad (60)$$

and these are the equations of the particles valid when they are considered separately.

Thus (54) satisfies the conditions laid down.

If the system is composed of  $N$  particles acting upon one another but not subject to constraints we can build up the generalised space by the  $3N$  rectangular co-ordinates and the  $\mu_{ik}$  and  $\mu^{ik}$  have the values (57). The wave equation takes the form :

$$\sum_i \frac{1}{m_i} \left( \frac{\partial^2 \psi}{\partial x_i^2} + \frac{\partial^2 \psi}{\partial y_i^2} + \frac{\partial^2 \psi}{\partial z_i^2} \right) - \frac{8\pi^2}{h^2} F \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t}, \quad (61)$$

where  $F$  now depends upon the  $3N$  variables  $x_1, x_2, \dots, z_N$  and the time  $t$ .

All these formulæ are non-relativistic, and it has not yet been possible to find a wave equation fulfilling the requirements of the theory of relativity. Moreover, we have, in agreement with Schrödinger's work, considered wave propagation in the fictitious generalised space. It has not yet been possible to connect this propagation of a single wave in a fictitious space with that of one or several waves in ordinary space.

This impossibility seems to strengthen the view that no physical reality is to be attached to the associated wave, but that it is simply a symbolic representation of probability.

## CHAPTER XV

### THE INTERPRETATION OF THE WAVE ASSOCIATED WITH THE MOTION OF A SYSTEM

#### 1. The Approximation of Geometrical Optics

**I**N order to explain the meaning of the many-dimensional wave associated with a system we begin with the wave equation :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial \psi}{\partial q_k} \right) - \frac{8\pi^2}{h^2} F \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} \quad (1)$$

We shall write  $\psi$  in the form  $ae^{\frac{2\pi i}{h}\phi}$ , when by substitution in (1) and equating the real and imaginary parts to zero, we find :

$$\frac{1}{2} \sum_{ik} \mu^{ik} \frac{\partial \phi}{\partial q_i} \frac{\partial \phi}{\partial q_k} + F = \frac{\partial \phi}{\partial t} + \frac{h^2}{8\pi^2 a} \frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a}{\partial q_k} \right), \quad (2)$$

$$\sum_{ik} \mu^{ik} \frac{\partial a}{\partial q_i} \frac{\partial \phi}{\partial q_k} + \frac{1}{2} \frac{a}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial \phi}{\partial q_k} \right) = \frac{\partial a}{\partial t}. \quad (3)$$

In the present section of this chapter we shall neglect the last term of (2), since we are limiting ourselves to the approximation of geometrical optics. The function  $\phi$  then satisfies Jacobi's equation, as we have seen, and we may regard the classical mechanics as valid in this case and define the Lagrangian momenta by :

$$p_i = \sum_k \mu_{ik} \dot{q}_k = - \frac{\partial S}{\partial q_i} = - \frac{\partial \phi}{\partial q_i}. \quad (4)$$

By solving these equations for the  $\dot{q}$ 's we find :

$$\dot{q}_i = \sum_k \mu^{ik} p_k = - \sum_k \mu^{ik} \frac{\partial \phi}{\partial q_k}. \quad (5)$$

By substitution in (3) :

$$\frac{\partial a}{\partial t} + \sum_i \frac{\partial a}{\partial q_i} \dot{q}_i + \frac{a}{2\sqrt{\mu}} \sum_i \frac{\partial}{\partial q_i} (\sqrt{\mu} \dot{q}_i) = 0 \quad . \quad (6)$$

and after multiplication by  $2a$  :

$$\frac{\partial a^2}{\partial t} + \frac{1}{\sqrt{\mu}} \sum_i \frac{\partial}{\partial q_i} (\sqrt{\mu} a^2 \dot{q}_i) = 0. \quad . \quad . \quad (7)$$

We shall interpret this equation in the same way as we interpreted that for a single particle.

We know that  $\phi$  satisfies Jacobi's equation to our degree of approximation. Let  $\phi = \phi(q_1, \dots, q_n, t, \alpha_1 \dots \alpha_n)$ ; according to Jacobi's theory the classical equations of motion are :

$$\frac{\partial \phi}{\partial \alpha_i} = \beta_i \quad (i = 1, 2, \dots, n). \quad . \quad . \quad (8)$$

To a particular function  $\phi$  with the same set of constants  $\alpha_i$ , there corresponds an infinity of possible motions dependent upon the choice of the constants  $\beta_i$ . We shall again describe these motions as being of the same class. The motion of the whole system is defined by the motion of its representative point in generalised space, and this motion is determined by the equations (8). Instead of considering a system, we can consider an assembly of identical systems performing motions of the same class and to this assembly there will correspond a cloud of points in the generalised space associated with the same  $\psi$ -wave. The velocities of these representative points are given by the equations (5).

The motion of this cloud of points must satisfy the hydrodynamical equation of continuity of which it is easy to find an explanation in the generalised space. Let us consider a small volume bounded by the surfaces :

$$q_i = c_i, \quad q_i = c_i + dq_i, \quad (i = 1, 2, \dots, n) \quad (9)$$

The sides of this small parallelepiped are in the directions of the co-ordinate axes  $q_i$ , and are of lengths  $dq_i$ . Consider a particular co-ordinate  $q_k$ . The number of representative points which cross the face  $q_k = c_k$  in time  $dt$  is equal to the number contained in an element with this face as base and with side

$\dot{q}_k dt$ . If  $\rho$  denote the density of the cloud at the face considered the flux is :

$$\sigma = \rho \sqrt{\mu} dq_1 \dots dq_{k-1} dq_{k+1} \dots dq_n \dot{q}_k dt \quad . \quad (10)$$

The flux across the parallel face  $q_k = c_k + dq_k$  is in the same way :

$$\sigma + \frac{\partial \sigma}{\partial q_k} dq_k$$

and the difference is :

$$- \frac{\partial}{\partial q_k} (\rho \sqrt{\mu} \dot{q}_k) dq_1 \dots dq_n dt. \quad . \quad (11)$$

In the same way, by considering each face of the parallelepiped, we obtain for the excess of the cloud entering over that which leaves the element the quantity :

$$- \sum_k \frac{\partial}{\partial q_k} (\rho \sqrt{\mu} \dot{q}_k) dq_1 \dots dq_n dt. \quad . \quad (12)$$

Expressed as a change of density this may also be written  $\frac{\partial \rho}{\partial t} dt \sqrt{\mu} dq_1 \dots dq_n$  and by equating the two expressions we obtain the equation of continuity :

$$\frac{\partial \rho}{\partial t} + \frac{1}{\sqrt{\mu}} \sum_k \frac{\partial}{\partial q_k} (\sqrt{\mu} \rho \dot{q}_k) = 0. \quad . \quad (13)$$

A comparison of (13) with (7) leads us to write :

$$\rho = K a^2 \quad . \quad . \quad . \quad (14)$$

This result may be expressed in terms of probability by considering a system of  $n$  degrees of freedom, the motion of which is known to belong to a certain class, but of which the initial configuration is not exactly known. The intensity of the associated wave in the generalised space measures at each point of the space the probability of occurrence of the representative point of the system.

The cloud of representative points may be replaced by a probability fluid of which the elements describe the various trajectories which are possible, according to the old dynamics, for the representative point, the density of the fluid being

proportional to  $a^2$  and being a measure of the probability of occurrence at each point of the space. It is thus possible to the approximation of geometrical optics to satisfy the principle of interference and at the same time to retain the view that the particles of the system have a definite position in space, and in consequence that the representative point itself has a definite position at each instant in the generalised space. For systems as for single particles the difficulties begin when we leave the realm of geometrical optics.

## 2. The General Case. Motion of Probability

When the approximations of the last paragraph cease to be valid, we can no longer neglect the last term in equation (2). The principle of interference will still be adopted according to which the square of the amplitude of the wave is a measure of the probability of occurrence of the representative point at each point of the space and at each instant. It will thus be necessary to associate a probability cloud with the  $\psi$ -wave, and the motion of the cloud in the space will be such that the principle of interference is satisfied. This result is attained by defining the velocity of the probability elements by the relations:

$$\dot{q}_i = - \sum_k \mu^{ik} \frac{\partial \phi}{\partial q_k}. \quad (15)$$

The equation of continuity is still satisfied on account of (3) by writing  $\rho = a^2$ .

The motion of the probability elements defined by (15) can be studied as in Chapter IX. Equation (2), which takes the place of Jacobi's equation, may be written :

$$\frac{1}{2} \sum_{ik} \mu^{ik} \frac{\partial \phi}{\partial q_i} \frac{\partial \phi}{\partial q_k} + F + F_1 = \frac{\partial \phi}{\partial t}, \quad (16)$$

where

$$F_1 = - \frac{h^2}{8\pi^2 a} \frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a}{\partial q_k} \right). \quad (17)$$

We can say that the probability elements move in the same way as if there were a supplementary potential energy of magnitude  $F_1$ , which may be described as quantum potential,

and which depends upon the amplitude  $a$  of the wave, and hence upon the density of the probability cloud. We may define a function of the  $q$ 's,  $\dot{q}$ 's and  $t$  by the formula :

$$L = \frac{1}{2} \sum_{ik} \mu_{ik} \dot{q}_i \dot{q}_k - F - F_1, \quad . \quad . \quad (18)$$

described as the Lagrangian function of the probability elements. The derivatives

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \sum_{ik} \mu_{ik} \dot{q}_k \quad . \quad . \quad (19)$$

are the conjugate momenta of the elements corresponding to the variables  $q_i$ .

By (15) we have :

$$p_i = - \sum_{kj} \mu_{ik} \mu^{kj} \frac{\partial \phi}{\partial q_j} = - \frac{\partial \phi}{\partial q_i} \quad . \quad . \quad (20)$$

and the quantity

$$W = \sum_i p_i \dot{q}_i - L = \frac{1}{2} \sum_{ik} \mu_{ik} \dot{q}_i \dot{q}_k - F - F_1 \quad . \quad (21)$$

plays the part of the energy.

We shall determine the equations of motion as in Chapter IX for the probability elements by calculating  $\frac{dp_i}{dt}$ .

$$\begin{aligned} \frac{dp_i}{dt} &= \sum_k \frac{\partial p_i}{\partial q_k} \dot{q}_k + \frac{\partial p_i}{\partial t} = \sum_{kj} \mu^{kj} \frac{\partial \phi}{\partial q_j} \frac{\partial^2 \phi}{\partial q_i \partial q_k} - \frac{\partial^2 \phi}{\partial q_i \partial t} \\ &= \frac{\partial}{\partial q_i} \left( \sum_{kj} \frac{1}{2} \mu^{kj} \frac{\partial \phi}{\partial q_k} \frac{\partial \phi}{\partial q_j} - \frac{\partial \phi}{\partial t} \right) - \frac{1}{2} \sum_{kj} \frac{\partial \mu^{kj}}{\partial q_i} \frac{\partial \phi}{\partial q_k} \frac{\partial \phi}{\partial q_j}, \end{aligned} \quad (22)$$

whence by (2), (19) and (20)

$$\frac{dp_i}{dt} = - \frac{\partial}{\partial q_i} (F + F_1) - \frac{1}{2} \sum_{kj} \frac{\partial \mu^{kj}}{\partial q_i} \sum_l \mu_{jl} \dot{q}_l \sum_m \mu_{km} \dot{q}_m, \quad (23)$$

but

$$\sum_j \mu^{kj} \mu_{jl} = \begin{cases} 0 & \text{if } k \neq l \\ 1 & \text{if } k = l \end{cases} \quad \sum_j \frac{\partial \mu^{kj}}{\partial q_i} \mu_{jl} = - \sum_j \mu^{kj} \frac{\partial \mu_{jl}}{\partial q_i} \quad (24)$$

and formula (23) is then written :

$$\frac{dp_i}{dt} = \frac{1}{2} \sum \mu^{kj} \frac{\partial \mu_{jl}}{\partial q_i} \mu_{km} \dot{q}_l \dot{q}_m - \frac{\partial}{\partial q_i} (F + F_1)$$

(where the summation applies to  $j, k, l$  and  $m$ )

$$= \frac{1}{2} \sum_{jl} \frac{\partial \mu_{jl}}{\partial q_i} \dot{q}_j \dot{q}_l - \frac{\partial}{\partial q_i} (F + F_1). \quad (25)$$

Finally, by the definition (18) :

$$\frac{dp_i}{dt} = \frac{\partial L}{\partial q_i}, \quad (i = 1, 2, \dots, n), \quad (26)$$

which is the Lagrangian set of equations.

The term  $-\frac{\partial F}{\partial q_i}$  in (25) is the  $q_i$ -component of force in the ordinary sense.

The term  $\frac{1}{2} \sum_{jl} \frac{\partial \mu_{jl}}{\partial q_i} \dot{q}_j \dot{q}_l$  is introduced by the choice of co-ordinates, and corresponds to centrifugal forces and forces of constraint. Both these terms occur in the equations of motion of ordinary mechanics and, if one may neglect  $-\frac{\partial F_1}{\partial t}$ , the motions of the probability elements in the generalised space are identical with the motions of the same class of representative points in classical dynamics. If, however,  $-\frac{\partial F_1}{\partial t}$  may not be neglected the elements move as if subject to an additional force derived from the quantum potential  $F_1$ . Thus, even in the absence of a force in the old classical sense, the principles of conservation of energy and of momentum do not hold for the probability elements.

### 3. Ehrenfest's Theorems

In the case of a system formed of  $N$  particles, subject to no constraints, we can eliminate the terms in  $F$  by means of an integration extended throughout the space and obtain once more theorems similar to those of Ehrenfest for a single particle (see Chapter IX, § 3).



We shall suppose the  $\psi$ -wave to be limited in the space in such a way that the amplitude  $a$  and its derivatives are zero at infinity and we begin with a mathematical result which generalises formula (21) of Chapter IX.

Let  $U$  and  $V$  be two functions of the co-ordinates  $q$ . Then if they be finite and continuous and vanish at infinity in the space, we shall have :

$$\int \frac{U}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial V}{\partial q_k} \right) d\tau = \int \frac{V}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial U}{\partial q_k} \right) d\tau, \quad (28)$$

where the integral is  $n$ -dimensional,  $d\tau$  being the element of volume in the  $n$ -dimensional space, and the integration is extended throughout the whole space.

For an account of the vanishing of  $U$  and  $V$  at infinity, the integral on the left can be transformed by partial integration as follows :

$$\begin{aligned} \int^{\mathbf{U}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu}^{-} \mu^{ik} \frac{\partial \mathbf{V}}{\partial q_k} \right) dq_1 \dots dq_n &= - \int \sqrt{\mu}^{-} \sum_{ik} \mu^{ik} \frac{\partial \mathbf{V}}{\partial q_k} \frac{\partial \mathbf{U}}{\partial q_i} dq_1 \dots dq_n \\ &= \int^{\mathbf{V}} \sum_{ik} \frac{\partial}{\partial q_k} \left( \sqrt{\mu}^{-} \mu^{ik} \frac{\partial \mathbf{U}}{\partial q_i} \right) dq_1 \dots dq_n \\ &= \int \frac{\mathbf{V}}{\sqrt{\mu}^{-}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu}^{-} \mu^{ik} \frac{\partial \mathbf{U}}{\partial q_k} \right) d\tau \quad (29) \end{aligned}$$

and (28) is thus established.

We shall describe the quantity :

$$\bar{f} = \int f a^2 d\tau \quad . \quad . \quad . \quad . \quad (30)$$

as the mean value of the function  $f$  in the probability cloud at time  $t$ . If we suppose that the system is without constraints we can choose for the  $q$  co-ordinates the  $3N$  rectangular co-ordinates of the system, and we have then :

$$\begin{aligned} \mu_{ik} &= \mu^{ik} = 0 \text{ if } i \neq k, \quad \mu_{jj} = \frac{1}{\mu^{jj}} = m_i \text{ for } j = 3i - 2, 3i - 1, 3i, \\ \mu &= (m_1 m_2 \dots m_N)^3, \end{aligned} \tag{31}$$

the quantity  $m_i$  being the mass of the  $i$ th particle. Since the  $\mu_{ik}$  are constants, the equations of motion of the probability (25) reduce to :

$$\frac{dp_i}{dt} = -\frac{\partial F}{\partial q_i} - \frac{\partial F_1}{\partial q_i} = f_i + \frac{\hbar^2}{8\pi^2} \frac{\partial}{\partial q_i} \left\{ \frac{1}{a\sqrt{\mu}} \sum_{kl} \frac{\partial}{\partial q_k} \left( \sqrt{\mu} \mu^{kl} \frac{\partial a}{\partial q_l} \right) \right\}. \quad (32)$$

In this equation we have taken account of the definition (17) of  $F_1$  and have denoted the  $q_i$ -component of the force in the classical sense by  $f_i$ .

If we multiply (32) by  $a^2 d\tau$  and integrate throughout the space we obtain :

$$\frac{d\bar{p}_i}{dt} = \bar{f}_i + \frac{\hbar^2}{8\pi^2} \int a^2 \frac{\partial}{\partial q_i} \left\{ \frac{1}{a\sqrt{\mu}} \sum_{kl} \frac{\partial}{\partial q_k} \left( \sqrt{\mu} \mu^{kl} \frac{\partial a}{\partial q_l} \right) \right\} d\tau. \quad (33)$$

The integral in this expression vanishes, for on account of (31) it can be written :

$$\begin{aligned} \int a^2 \frac{\partial}{\partial q_i} \left( \frac{1}{a} \sum_k \mu^{kk} \frac{\partial^2 a}{\partial q_k^2} \right) d\tau &= \int \left\{ a \frac{\partial}{\partial q_i} \left( \sum_k \mu^{kk} \frac{\partial^2 a}{\partial q_k^2} \right) - \frac{\partial a}{\partial q_i} \sum_k \mu^{kk} \frac{\partial^2 a}{\partial q_k^2} \right\} d\tau \\ &= \int \left( a \sum_k \mu^{kk} \frac{\partial^3 a}{\partial q_i \partial q_k^2} - \frac{\partial a}{\partial q_i} \sum_k \mu^{kk} \frac{\partial^2 a}{\partial q_k^2} \right) d\tau \end{aligned} \quad (34)$$

and (28) gives by virtue of (31) :

$$\int U \sum_k \mu^{kk} \frac{\partial^2 V}{\partial q_k^2} d\tau = \int V \sum_k \mu^{kk} \frac{\partial^2 U}{\partial q_k^2} d\tau. \quad (35)$$

In this formula write  $U = a$ ,  $V = \frac{\partial a}{\partial q_i}$ , since  $a$  and its derivatives satisfy the conditions imposed upon  $U$  and  $V$  in the development of (28), and it follows immediately that the right-hand side of (34) vanishes. (33) now gives :

$$\frac{d\bar{p}_i}{dt} = \bar{f}_i, \quad (i = 1, 2, \dots N). \quad (36)$$

If there is no external field of force or if the external field is independent of the time, a theorem analogous to that of the conservation of energy may be established. It may be shown, as in the preceding chapter, by means of the definition (21) of the energy of the probability elements, that :

$$\frac{dW}{dt} = -\frac{\partial L}{\partial t} = \frac{\partial F}{\partial t} + \frac{\partial F_1}{\partial t}. \quad (37)$$

After multiplying by  $a^2$  and integrating throughout the space, it is found that :

$$\frac{d\overline{W}}{dt} = \frac{\partial \overline{F}}{\partial t} - \frac{h^2}{8\pi^2} \int a^2 \frac{\partial}{\partial t} \left\{ \frac{1}{a\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a}{\partial q_k} \right) \right\} d\tau \quad (38)$$

and the integral may be written :

$$\int a^2 \frac{\partial}{\partial t} \left( \frac{1}{a} \sum_k \mu^{kk} \frac{\partial^2 a}{\partial q_k^2} \right) d\tau = \int \left( a \sum_k \mu^{kk} \frac{\partial^3 a}{\partial q_k^2 \partial t} - \frac{\partial a}{\partial t} \sum_k \mu^{kk} \frac{\partial^2 a}{\partial q_k^2} \right) d\tau. \quad (39)$$

If the same substitutions be made for  $U$  and  $V$  as above, we obtain from (38) :

$$\frac{d\overline{W}}{dt} = \frac{\partial \overline{F}}{\partial t}, \quad . \quad . \quad . \quad . \quad (40)$$

and in the case when the external field is independent of the time,  $\frac{\partial \overline{F}}{\partial t}$  is zero and therefore :

$$\frac{d\overline{W}}{dt} = 0. \quad . \quad . \quad . \quad . \quad (41)$$

This is the theorem in the case of elements of probability which replaces that of conservation of energy.

#### 4. The Explanation of Bohr and Heisenberg

Here, as in the case of the single particle, we might be tempted to develop a pilot-wave theory, at the same time maintaining that the particles of the system have a definite position in space and that, consequently, the representative point has also a definite position at each instant in the generalised space. We should then admit that the representative point associated with a  $\psi$ -wave has the motion defined by (15), coinciding always with one of the probability elements. If we do not know with which of the probability elements the point coincides, the probability that it occupies a volume  $d\tau$  at time  $t$  will be equal to the number of elements then contained within the volume and by (14) the interference principle will be automatically satisfied. Unfortunately all the difficulties arise once more which we discovered in the pilot-wave theory of a particle, and it is even more difficult to consider the theory as offering an actual physical picture of the phenomena because

of the abstract and fictitious character of the propagation of a wave in generalised space.

We therefore leave the pilot-wave theory and turn to that of Bohr and Heisenberg to see how it will apply to systems. We shall accept as fundamental hypotheses the interference principle, according to which the intensity  $\psi\psi^*$  of the associated wave measures at each instant and at each point the probability of occurrence of the representative point, and the principle of spectral decomposition, according to which the relative intensities of the different monochromatic components of which the  $\psi$ -wave train is composed give the relative probabilities of the different states of motion. All the considerations developed in the case of a single particle may be extended to the case of  $N$  particles and the uncertainty relations again obtained :

$$\delta q_i \delta p_i \geq h. \quad . \quad . \quad . \quad (42)$$

The cause of this uncertainty is always to be sought in the perturbation introduced of necessity in the process of measurement.

The transition from the old to the new mechanics conceived after the manner of Bohr and Heisenberg can also be made by means of Ehrenfest's theorem, as in Chapter XI. When geometrical optics is valid for the propagation of the wave in generalised space trains of waves may exist occupying a region of dimensions large compared with the wave-length and which can, therefore, be represented by a group of nearly monochromatic waves. Although comprising many wave-lengths, these trains may on our scale still be considered of negligible dimensions, and they may be compared with a small probability element in the space. Within such an element the quantities  $p_i$  and  $-\frac{\partial F}{\partial q_i}$  are appreciably constant, and Ehrenfest's theorem then gives :

$$\frac{dp_i}{dt} = -\frac{\partial F}{\partial q_i}. \quad . \quad . \quad . \quad (43)$$

Thus the probability element moves as a whole in the space like the representative point in the classical theory. The position of this point must, of course, be regarded as indeterminate within the element, but this indeterminateness is so small on our scale that it can be neglected in practice. Actually it

appears as if the configuration and state of motion were exactly defined at any instant and as if the system followed rigorously the laws of the old mechanics.

### 5. Concluding Remark

We make a last remark on this subject in the case where the system consists of particles exercising no action upon one another. From the last chapter it appears that we must take for  $\psi$  the product of the functions for the different particles considered separately,  $\psi = \psi_1 \psi_2 \dots$ . This is in agreement with the interference principle and with the statistical meaning of intensity. For the probability that the representative point of the system shall occupy the position  $(x_1, y_1, \dots, z_N)$  at time  $t$  is :

$$\psi(x_1, y_1, \dots, z_N, t) \psi^*(x_1, y_1, \dots, z_N, t) \quad . \quad (44)$$

and the probability that the  $i$ th particle is at  $(x_i, y_i, z_i)$  at this instant is :

$$\psi_i(x_i, y_i, z_i, t) \psi_i^*(x_i, y_i, z_i, t), \quad . \quad . \quad (45)$$

but since the motions of the particles are independent, there being no mutual action, the probability that the particles will occur simultaneously at the corresponding points is  $\prod \psi_i \psi_i^*$ .

This is equal to  $\psi \psi^*$ , since

$$\psi = \prod \psi_i. \quad . \quad . \quad . \quad . \quad (46)$$

## CHAPTER XVI

### THE OLD QUANTUM THEORY AND THE STABILITY OF PERIODIC MOTION

#### 1. Early Examples of Quantisation in Periodic Motion

**I**N atomic phenomena periodic motion plays a great part, and we must study the special characteristics of this type of motion in wave mechanics. We shall begin by recalling how the conception of a quantum of action was introduced into the study of periodic phenomena in the atom and point out some of the chief results of the old quantum theory.

It is well known that the idea of the quantum was introduced into dynamics by Planck in his researches into the state of thermodynamical equilibrium between matter and radiation. As this state cannot depend upon the mechanism of the energy exchange he assumed, for the sake of simplicity, that it was brought about by means of electrons vibrating about a position of equilibrium to which they were attracted by a force proportional to the displacement. A particle of this kind oscillating in a straight line under this law of force is called a linear oscillator. In order to obtain the experimental laws of complete radiation Planck was led to make the assumption that the oscillators could not be in possession of arbitrary amounts of energy, but that only those amounts were permissible which were related to the frequency of oscillation by the formula :

$$E = nh\omega, \quad . \quad . \quad . \quad . \quad . \quad (1)$$

$n$  being an integer,  $h$  the constant of action introduced by Planck into physics, and  $\omega$  the frequency of the oscillator, which, as we shall show, is independent of the energy.

We can obtain another expression of this quantum postulate

from a consideration of the linear oscillator. The potential function,  $F$ , is :

$$F = \frac{k}{2}x^2, \quad . \quad . \quad . \quad . \quad (2)$$

$x$  being the displacement, and the classical equation of motion is :

$$m \frac{d^2x}{dt^2} = -kx. \quad . \quad . \quad . \quad (3)$$

The solution is :

$$x = A \sin \left( \sqrt{\frac{k}{m}}t + \alpha \right), \quad . \quad . \quad . \quad (4)$$

where  $A$  and  $\alpha$  are two arbitrary constants.

The frequency

$$\omega = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \quad . \quad . \quad . \quad (5)$$

is independent of  $A$ , the energy of the motion.

The momentum is  $p_x = m \frac{dx}{dt} = mv$ , and the integral of action of Maupertuis is :

$$S_1 = \int_{x_0}^{x_1} p_x dx = m \int_{x_0}^{x_1} v dx \quad . \quad . \quad . \quad (6)$$

and if this be calculated for a complete period we find :

$$\begin{aligned} J &= \oint dS_1 = \oint mv dx = m \int_0^{\frac{1}{\omega}} v^2 dt \\ &= 2\pi^2 \omega m A^2 \quad . \quad . \quad . \quad (7) \end{aligned}$$

by (4).

The energy,  $E$ , is equal to the kinetic energy of the particle at the instant it passes through the position of equilibrium, since at this point the potential energy is zero.

Thus :

$$E = \frac{1}{2} m \dot{x}_0^2 = \frac{1}{2} k A^2 = 2\pi m \omega^2 A^2, \quad . \quad . \quad (8)$$

whence

$$\frac{E}{\omega} = 2\pi m \omega A^2 = J. \quad . \quad . \quad (9)$$

The condition (1) may be written in the form :

$$J = n\hbar, \quad . \quad . \quad . \quad (10)$$

but this is much more general, since it is not necessary to make the special assumption that the frequency of the oscillator is independent of its energy. Moreover, the quantum restriction of energy values for all motion with one degree of freedom can be expressed in this form. The condition (10) is the condition of quantisation.

The most important application of (10) is that made by Bohr to the case of an electron of charge  $-e$  rotating about a positive nucleus of charge  $+e$ , as in the atom of hydrogen. In his first work on this subject in 1913 Bohr limited himself to the study of circular trajectories. The azimuth  $\theta$  is in this case the only variable necessary for locating the particle and (10) can be applied. The kinetic energy is :

$$T = \frac{1}{2}mr^2\dot{\theta}^2 \quad . \quad . \quad . \quad (11)$$

and the momentum conjugate to  $\theta$  is :

$$p_\theta = \frac{\partial T}{\partial \dot{\theta}} = mr^2\dot{\theta}, \quad . \quad . \quad . \quad (12)$$

hence the integral of action is :

$$\int p_\theta d\theta = \int mr^2\dot{\theta} d\theta. \quad . \quad . \quad . \quad (13)$$

Since the angular velocity  $\dot{\theta}$  is constant on a circular path in a central field of force the value of the integral for a complete period is :

$$J = \int_0^{2\pi} mr^2\dot{\theta} d\theta = 2\pi mr^2\dot{\theta}. \quad . \quad . \quad (14)$$

Condition (10) becomes in this case :

$$2\pi mr^2\dot{\theta} = nh. \quad . \quad . \quad . \quad (15)$$

$mr^2\dot{\theta}$  is the moment of momentum of the electron with respect to the nucleus, and if this be denoted by  $M$ , (15) may be written :

$$M = \frac{nh}{2\pi}, \quad . \quad . \quad . \quad (16)$$

which is the formula which led Bohr to his brilliant explanation of the hydrogen spectrum. To obtain the formula for this spectrum we may write the equation of motion in the form :

$$mr\dot{\theta}^2 = \frac{e^2}{r^2}, \quad . \quad . \quad . \quad (17)$$



and eliminating  $\dot{\theta}$  between (16) and (17) we obtain :

$$\frac{1}{r} = \frac{4\pi^2 m e^2}{n^2 h^2}. \quad (18)$$

The energy of the electron in its path is :

$$E = \frac{1}{2} m r^2 \dot{\theta}^2 - \frac{e^2}{r} = - \frac{e^2}{2r}, \quad (19)$$

whence

$$E_n = - \frac{2\pi^2 m e^4}{n^2 h^2}. \quad (20)$$

This is the well-known formula for the energies in the various quantum states for the hydrogen atom.

At this point Bohr introduced another postulate known as the law of frequencies, according to which the atom emits radiation of frequency  $\nu_{nm}$  when it passes from one stable quantum state with energy  $E_n$  to another with less energy  $E_m$ , the frequency being given by :

$$\nu_{nm} = \frac{E_n - E_m}{h} = \frac{2\pi^2 m e^4}{h^3} \left( \frac{1}{m^2} - \frac{1}{n^2} \right). \quad (21)$$

If  $m$  is made equal to 2, that is if all those changes of state are considered which terminate in a final state characterised by this number, the experimental formula for the Balmer series is obtained :

$$\nu = R \left( \frac{1}{4} - \frac{1}{n^2} \right). \quad (n = 3, 4, \dots). \quad (22)$$

If the two formulæ are identical it must follow that :

$$R = \frac{2\pi^2 m e^4}{h^3}. \quad (23)$$

and the great success of Bohr's theory is that the experimental value of  $R$  agrees with formula (23).

Equation (21) gives the frequencies of the members of another series in the hydrogen spectrum known as the Lyman and Paschen series, and from a consideration of the circular orbits of an electron about a doubly charged nucleus, Bohr has also succeeded in explaining the spectrum of ionised helium.

## 2. The Wilson-Sommerfeld Conditions

The satisfactory enunciation of the quantum conditions in the periodic motion of a particle in a constant field of force required an extension beyond the case where the motion is defined by a single variable. W. Wilson and Sommerfeld found a form of enunciation applicable to all periodic motion where there is separation of the variables, that is to say, where it is possible to choose the co-ordinates in such a way that each conjugate component of momentum depends only upon the corresponding co-ordinate :

$$p_i = f(q_i). \quad . \quad . \quad . \quad . \quad (24)$$

The action of Maupertuis,  $\int \sum_i p_i dq_i$ , is thus a sum of functions each of which depends upon a single variable. It may be shown that, in the course of the motion, some of the variables oscillate between two limits, while the others are angles with a period  $2\pi$ . For example, in Keplerian motion the radius vector is a variable of the first kind, the azimuth one of the second. We shall say that a variable of the first kind has completed its cycle when it has increased from the lower to the upper limit and has returned to the lower ; in the same way we shall say that a variable of the second kind has described its cycle when it has increased by  $2\pi$ . With these definitions in mind we can pass on to state the quantum conditions of Wilson and Sommerfeld. The variables,  $q_i$ , having been chosen so that the variables can be separated, each of the integrals  $\int p_i dq_i$  taken over a complete cycle of  $q_i$  is equal to an integral multiple of the constant  $h$ . The conditions may be written :

$$\oint p_i dq_i = n_i h. \quad (n_i = \text{an integer.}) \quad . \quad . \quad (25)$$

A particle in motion in a constant field of force has, in general, three degrees of freedom and will require, in general, three integers for the definition of its quantised motion.

We may note an important point. When  $q_i$  is a variable of the first kind like the radius vector in the Kepler problem,

it oscillates during the motion between values  $q_{i0}$  and  $q_{i1}$  and the integral in this case is :

$$\int_{q_{i0}}^{q_{i1}} p_i dq_i + \int_{q_{i1}}^{q_{i0}} p_i dq_i. \quad . \quad . \quad . \quad (26)$$

This integral would clearly be zero if  $p_i$  were a uniform function of the variable  $q_i$ ; but this is not the case, for it can be shown that in the motion with which we are concerned the conjugate momentum of a variable of the first kind is of the form :

$$p_i = \pm \sqrt{\phi_i(q_i)}, \quad . \quad . \quad . \quad (27)$$

the function  $\phi_i$  being positive in the interval  $q_{i0}$  to  $q_{i1}$ , and vanishing at the limits and then changing sign.  $p_i$  is thus a

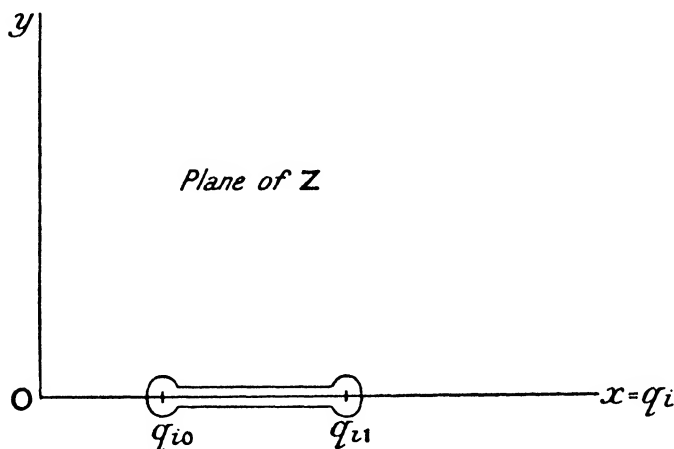


FIG. 13.

double valued function of  $q_i$ , and we must of course take the positive sign in (27) when  $q_i$  is increasing and the negative sign when it is decreasing so that the integral may be positive.

We can express this by the use of the complex variable  $z$ , of which  $q_i$  is the real part. Let a function  $p_i$  be defined by the formula :

$$p_i = \pm \sqrt{\phi_i(z)}. \quad . \quad . \quad . \quad (28)$$

Along the real axis this expression is identical with (27) and  $p_i$  is the momentum conjugate to  $q_i$ . The function has two branch points on the real axis and the integral must be taken

along a closed contour extending from the position  $q_{i0} + \epsilon$  to  $q_{i1} - \epsilon$  on the real axis and completed by two infinitely small circles of radii  $\epsilon$  about the branch points (Fig. 13).

There is no corresponding process for the variables of the second kind which vary from 0 to  $2\pi$ ; for these the momentum has a constant sign.

### 3. Einstein's Statement of the Quantum Conditions

The Wilson-Sommerfeld conditions can be stated independently of the choice of variables in a form given by Einstein in 1917.

In the case of a particle the action is given by :

$$dS_1 = \sum_1^3 p_i dq_i.$$

This expression is invariant for any change of space co-ordinates, for it represents what may be described as the work of the momentum vector. Throughout the region R, where the motion takes place, each component  $p_k = \frac{\partial S_1}{\partial q_k}$  is in general a function of the three variables, for we are no longer limiting ourselves to co-ordinates which are separable. The quantum conditions are equivalent to the statement that the integral of action, taken over any closed curve C situated wholly within R, is equal to an integral multiple of Planck's constant.

To calculate this integral it is necessary to choose a system of co-ordinates, for example one in which the variables are separable. We can then write :

$$\int_C dS_1 = k_1 \int p_1 dq_1 + k_2 \int p_2 dq_2 + k_3 \int p_3 dq_3. \quad (29)$$

$k_1$ ,  $k_2$  and  $k_3$  being integers and by virtue of the conditions (25) Einstein's statement is satisfied. The Wilson-Sommerfeld conditions thus lead to Einstein's form, but the latter is independent of the choice of co-ordinates.

As an illustration of this principle of Einstein's let us consider a motion taking place in a plane under the action of a central force. The radius vector, being a variable of the first

kind, oscillates between two values  $r_1$  and  $r_2$ , and in general the plane orbit fills the annular region included between the circles of radii  $r_1$  and  $r_2$ .

The continuous line denotes the plane of the orbit (Fig. 14). The motion may be described by means of the azimuth  $\theta$  measured about O and the radius vector  $r$ ; to these correspond the conjugate momenta  $p_\theta$  and  $p_r (= \pm \sqrt{\phi(r)})$ . Let us imagine the annular area to be replaced by a surface formed of two plane sheets which have been bent to fit along the circles  $r = r_1$  and  $r = r_2$ , making in this way a Riemannian surface. The upper sheet will be associated with the positive, the lower with the negative sign. In Fig. 14 these sheets are represented

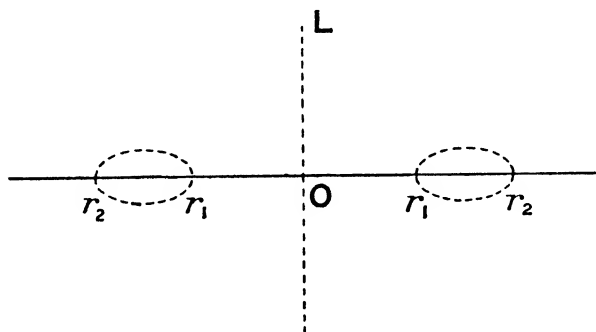


FIG. 14.

by dotted lines and for convenience they are shown displaced from one another. The annular area is thus replaced by a sort of flattened anchor ring on which  $p_r$  is a uniform function.

It is possible to distinguish three types of curves on this surface :—

1. Those which can be reduced to a point by a continuous change of shape. For these  $\int_C dS_1 = 0$ .
2. Those which can be made by a continuous deformation to coincide with a circle about the axis through O perpendicular to the plane of the ring and for which

$$\int_C dS_1 = \int_0^{2\pi} p_\theta d\theta = n_1 h.$$

3. Finally, those which can be made by a continuous deformation to coincide with a section of the surface by a plane containing the axis and for which

$$\int_C dS_1 = \oint p_r dr = n_2 h.$$

Moreover, any curve traced on the Riemann surface can be referred to a series of curves of these three types and Einstein's enunciation results.

#### 4. Quantisation of Keplerian Motion

As an example of the application of the quantum conditions we will consider the case of Keplerian motion.

In polar co-ordinates the classical kinetic energy is :

$$T = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) \quad . \quad . \quad . \quad (30)$$

and the conjugate momenta are :

$$p_r = \frac{\partial T}{\partial \dot{r}} = m\dot{r}, \quad p_\theta = \frac{\partial T}{\partial \dot{\theta}} = mr^2\dot{\theta}. \quad . \quad . \quad (31)$$

But by the law of areas  $p_\theta$  is equal to a constant C, and Newton's or Coulomb's law of force makes it possible to write :

$$E = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - \frac{K}{r}, \quad . \quad . \quad (32)$$

from which we may deduce by replacement of  $p_\theta$  by C :

$$p_r = m\dot{r} = \pm \sqrt{2mE - \frac{C^2}{r^2} + \frac{2mK}{r}} = \pm \sqrt{\phi(r)}. \quad (33)$$

If E is negative  $\phi$  has two positive roots  $r_1$  and  $r_2$  and the radius-vector must always be included between these roots if  $p_r$  is not to become imaginary. Thus if E is negative the motion is periodic and  $p_r$  is of the form (27).

The quantum condition for the azimuth is :

$$\int_0^{2\pi} p_\theta d\theta = 2\pi C = n_1 h, \quad (n_1 = \text{an integer}) \quad . \quad (34)$$

or

$$C = n_1 \frac{h}{2\pi}, \quad . \quad . \quad . \quad (35)$$

where  $n_1$  is called the azimuthal quantum number.

This is the condition of stability (16) used by Bohr in the case of circular motion, for  $C$  is the constant moment of momentum of the "planet" about the "sun."

But in the present case we have in addition a second quantum condition which Bohr did not require, since he restricted himself to circular orbits. This second condition is :

$$\oint p_r dr = n_2 h, \quad . \quad . \quad . \quad (36)$$

where  $n_2$  is the radial quantum number.

If  $r_1$  and  $r_2$  are the roots of  $\phi(r)$  the integral (36) may be written :

$$\int_{r_1}^{r_2} \sqrt{\phi} dr + \int_{r_2}^{r_1} -\sqrt{\phi} dr = 2 \int_{r_1}^{r_2} \sqrt{\phi} dr \quad . \quad (37)$$

and by equating this to  $n_2 h$  a second condition is obtained to which we shall return later on.

We can easily obtain, by a general process, expressions for the  $p_i$  in terms of the  $q_i$  which are required for the calculation of the integrals from Jacobi's equation. In the special case of Keplerian motion this may be shown by writing the energy (32) in the form :

$$H(q_i, p_i) = \frac{1}{2m} \left( p_r^2 + \frac{p_\theta^2}{r^2} \right) - \frac{K}{r}, \quad . \quad . \quad (38)$$

and Jacobi's equation for the function  $S_1$  is :

$$\frac{1}{2m} \left\{ \left( \frac{\partial S_1}{\partial r} \right)^2 + \frac{1}{r^2} \left( \frac{\partial S_1}{\partial \theta} \right)^2 \right\} - \frac{K}{r} = E. \quad . \quad (39)$$

Substituting  $\frac{\partial S_1}{\partial \theta} = C$ , we find :

$$p_r = \frac{\partial S_1}{\partial r} = \sqrt{2mE + \frac{2mK}{r} - \frac{C^2}{r^2}}. \quad . \quad (40)$$

The function  $S_1 = C\theta + \int p_r dr$  is a complete integral of (39), for it contains two arbitrary constants  $C$  and  $E$ , the values of these constants being determined by the quantum conditions (35) and (37).

### 5. Degeneration

We have to consider next a subject which has played a very important part in the old quantum theory ; this is the subject of degeneration. It was stated that the Wilson-Sommerfeld conditions characterised the quantised motion of a particle by means of three whole numbers. But from the results given above it follows that these three numbers intervene effectively only when three variables are necessary for the description of the motion. Bohr, in considering only circular motion described by a single variable, the azimuth, had to introduce only a single integer ; in the last paragraph, in the study of Keplerian motion which is plane and is described by means of a radius vector and an azimuth, we required only two integers,  $n_1$  and  $n_2$ .

But it is important to note that the occurrence of two numbers in Keplerian motion is only accidental. This becomes clear at once by noting that the orbit in the classical theory is a closed conic, and thus if elliptic co-ordinates are chosen the motion can be described by a single variable.

These results can be generalised in the statement that every time the trajectory, instead of filling the whole of a three-dimensional region, fills only a two-dimensional or a one-dimensional region, the process of quantisation introduces only two numbers or a single number. In this case we have degeneration.

The study of Keplerian motion confirms this conclusion, as we shall appreciate by completing the calculations begun in the last paragraph. By means of Cauchy's theory of residues Sommerfeld has obtained the value of the integral :

$$\oint p_r dr = \oint \sqrt{2mE + \frac{2mK}{r} - \frac{c^2}{r^2}} dr. \quad . \quad . \quad (41)$$

He has found the energy of the orbit characterised by the numbers  $n_1$  and  $n_2$  by equating the result to  $n_2 h$  and substituting the value  $\frac{n_1 h}{2\pi}$  for C. The result is :

$$E_{n_1 n_2} = - \frac{2\pi^2 m e^4}{h^2 (n_1 + n_2)^2}. \quad . \quad . \quad (42)$$

By making  $n_2 = 0$  we obtain again Bohr's result for circular orbits, but Sommerfeld's result shows that the energy of the quantised elliptic orbits is also characterised by a single integer,



$n_1 + n_2$ . The consideration of elliptic orbits does not introduce a single new term into the list of stable energy levels. The separate introduction of the two quantum numbers  $n_1$  and  $n_2$  appears therefore to be fictitious. This is shown better still by the fact that in the case of classical Keplerian motion it is possible to realise separation of the variables in other ways than by means of the radius vector and the azimuth. Each choice of variables which brings about separation of the variables leads to different forms for the stable elliptic orbits, but gives the same values for their energies. It must be concluded that all circular or elliptic orbits with energies equal to  $-\frac{2\pi^2 me^4}{n^2 h^2}$  are stable. Quantisation of Keplerian orbits brings in finally only a single integer because the orbits are closed, occupying only one dimension in space, and classical Keplerian motion is degenerate.

Degenerate motions present a special kind of instability in the sense that the least perturbation causes the degeneration to disappear, at least partially. Thus it is well known in astronomy that a perturbation, even a very feeble one, can impose periodic or secular variations on the elements of a Keplerian elliptic orbit (major axis, eccentricity, inclination, longitude of the perihelion, longitude of the ascending node), the consequence of these variations being that the orbit is no longer strictly closed and that it fills completely a space domain. The introduction of the relativity correction into the theory of Keplerian orbits is equivalent to introducing perturbation terms which are in general small, and Sommerfeld has shown that the orbit remains plane and appreciably elliptic, but that there is a slow continuous rotation of the perihelion. The trajectory is thus no longer exactly closed, and it occupies the whole of the annular area between two circles of radii equal to the distances from the attracting focus to the ends of the major axis of the rotating ellipse. The degeneration thus disappears, but only partially, since the trajectory remains plane, but it is now necessary to introduce two numbers for each stable orbit. By calculations which we will not reproduce here, Sommerfeld obtains for the energy of the quantised path characterised by the numbers  $n_1$  and  $n_2$ :

$$E_{n_1 n_2} = -\frac{2\pi^2 me^4}{n^2 h^2} \left\{ 1 + \frac{4\pi^2 e^4}{n^2 h^2 c^2} \left( \frac{n}{n_1} - \frac{3}{4} \right) \right\}, \quad (43)$$

where  $n = n_1 + n_2$  is the total quantum number. From this it is clear that the energy of the stable orbit depends separately upon the two numbers  $n_1$  and  $n_2$  and not only upon the sum  $(n_1 + n_2)$ .

An electric or magnetic field acting upon the hydrogen atom also causes the degeneration to disappear from the corresponding Kepler motion.

## 6. The Insufficiency of the Old Quantum Theory

It is impossible to examine all the calculations to which the various applications of the quantum conditions give rise. We must be content with remarking that although the calculations have often led to exact results it has not always been the case, and the old theory has more than once proved to be insufficient.

Let us return to the case of the linear oscillator treated in § 1. From the formula (1) the energy  $E$  of the stable states must be equal to one of the values of the series:  $0, \hbar\omega, 2\hbar\omega, \dots, n\hbar\omega$ , where  $\omega$  is the mechanical frequency,  $\frac{1}{2\pi} \sqrt{\frac{k}{m}}$  of the oscillator.

But in order to explain certain experiments, especially in the domain of band spectra, we have been obliged to admit that the sequence of quantised energies is not that we have just stated, but the following:

$$\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \dots, (n + \frac{1}{2})\hbar\omega. \quad (n = 0, 1, 2, \dots)$$

This is what is sometimes called the half quantum law and is not in agreement with the quantisation required by the old quantum theory. The application of the method of quantisation of the old theory to more complex atoms than those of hydrogen and helium has also led to poor results; for example, the ionisation potential of helium as calculated by Kramers according to the old methods is not in agreement with experiment.

For some time before the appearance of the new mechanics the impression had been formed that the Wilson-Sommerfeld conditions, while affording valuable indications, could not be considered as rigorous. We pass on now to see in what sense the new mechanics modifies these methods and how it has revealed to some extent the physical meaning of the quantum conditions.

## CHAPTER XVII

### THE STABILITY OF QUANTISED MOTION FROM THE POINT OF VIEW OF WAVE MECHANICS

#### 1. Meaning of Quantisation in Wave Mechanics

WE have been led by the conceptions of wave mechanics to associate with the motion of a particle in a constant field of force defined by the potential  $F(x, y, z)$  the propagation of a wave given by the equation :

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - F) \psi = 0. \quad . \quad . \quad (1)$$

If the approximations of geometrical optics are valid for the study of this wave propagation we can take as the reduced wave function :

$$\psi = ae^{\frac{2\pi i}{h}(Et - S_1)}, \quad . \quad . \quad . \quad (2)$$

where  $a$  depends upon  $x, y$  and  $z$  only and where  $S_1(x, y, z)$  is a complete integral of Jacobi's equation. In order that the phase of the function (2) may have a definite value at every point it is necessary and sufficient that along any closed curve  $C$  contained in the region of propagation we have :

$$\int_{C_1} dS_1 = \int_C \sum_1^3 p_i dq_i = nh. \quad (n = \text{an integer.}) \quad . \quad (3)$$

We thus obtain once more Einstein's result from which the Wilson-Sommerfeld conditions follow. In the special case of a closed trajectory we can take it as our closed curve  $C$  and write down the single condition :

$$\int p \, dl = nh. \quad . \quad . \quad . \quad (4)$$

The problem is then degenerate and each stable orbit is characterised by a single integer.

Thus if geometrical optics be valid for the propagation of the associated waves in the atoms the new mechanics gives a meaning to the mysterious quantum conditions. Since according to the new view geometrical optics and the old mechanics correspond, we can say that the quantum conditions in the old quantum theory are those which must be introduced in order to preserve the equations of the old mechanics. But this makes the whole of the old quantum theory appear nothing more than a first approximation valid within the same limits as geometrical optics. Now, as Schrödinger has pointed out, this approximation is insufficient in the case of intra-atomic motion. In fact, the essential condition of application of geometrical optics is that the conditions of propagation vary very little for displacements of the order of a wave-length, and since the wave-length of the wave associated with an electron in an atom is  $\frac{h}{mv}$ , or approximately  $\frac{7.3}{v}$ , with intra-atomic velocities of the order  $10^9$  cm. per sec., the order of magnitude ( $10^{-8}$  cm.) is that of the dimensions of the atom. Within the intra-atomic domain the conditions of propagation vary enormously, since they are governed by the potential  $F$  which increases indefinitely when the nucleus is approached. The application of the results of geometrical optics is thus not justified.

In short, the explanation of the old quantum conditions which we have just given puts us upon the track of the solution, but it shows also that these conditions cannot be considered as rigorous, and that the whole question of quantisation must be taken up again from the wave point of view. How shall we define a stable quantum state?

It is natural with the new ideas to suppose that a stable state corresponds to a  $\psi$ -wave having the form of a stationary wave :

$$\psi = a(x, y, z)e^{\frac{2\pi i}{h}(Et + \alpha)}. \quad . \quad . \quad . \quad (5)$$

Since  $\psi$  is a solution of (1) the amplitude must satisfy the equation :

$$\nabla^2 a + \frac{8\pi^2 m}{h^2}(E - F)a = 0. \quad . \quad . \quad (6)$$

We shall suppose that the amplitude is a finite, uniform and continuous function. Moreover, the interference principle leads

us to suppose it to vanish at infinity ; for if the amplitude did not tend to zero at infinity, the integral,  $\int a^2 dv$ , would be divergent, since all the elements of it are positive and the probability that the particle was situated at a finite distance from the atomic system considered would be zero. This would be contradictory to the idea that the particle forms part of the system and is in a stable state within it.

From the point of view of wave mechanics the search for the stable states of a particle becomes the problem of finding values of  $E$  for which the equation :

$$\nabla^2 a + \frac{8\pi^2 m}{h^2} (E - F) a = 0 . \quad . \quad . \quad (7)$$

has a solution which is uniform, finite and continuous everywhere and vanishes at infinity. The values of  $E$  defined in this way are the energies in the quantum states of the particle. The mathematical problem is closely analogous to that of determining the characteristic vibrations of a string or membrane when certain boundary conditions are imposed. In this case the boundary condition is that  $a$  must vanish at infinity.

To study the mathematical problem we have just stated we shall make use of the following notation :

$$\mu = \frac{8\pi^2 m E}{h^2}, \quad R = \frac{8\pi^2 m F}{h^2} . \quad . \quad . \quad (8)$$

Equation (7) is then written in the form :

$$\nabla^2 a + (\mu - R) a = 0 . \quad . \quad . \quad (9)$$

We shall show that this equation admits of solutions which are uniform, finite and continuous in a region  $D$  of space and which vanish at the boundaries of this region for certain values only of  $\mu$ . These special values are called the fundamental or characteristic constants of equation (9) and sometimes the proper values. In this way the existence of quantised values of the energy will be established.

In general a single solution of (9) corresponds to each proper value, fulfilling the conditions laid down ; this is the fundamental, characteristic or proper function corresponding to the particular value of  $\mu$ . We shall show that if  $a_i$  and  $\mu_i$  denote

two fundamental functions corresponding to two fundamental constants  $\mu_i$  and  $\mu_j$  then :

$$\int_D a_i a_j dv = 0. \quad . \quad . \quad . \quad (10)$$

In other words, the fundamental functions form an orthogonal system.

In order to grasp the physical character of this theory it is convenient to begin with the study of some simple classical cases of equations of the form (9) in which  $R = 0$ .

## 2. Simple Examples of Characteristic Vibrations. Vibrating Strings and Membranes

### (a) *The Case of a String with Fixed Ends.*

In the propagation of an elastic wave along a string fixed at both ends, the transverse displacement  $u$  of a point of the string satisfies the wave equation :

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{V^2} \frac{\partial^2 u}{\partial t^2}, \quad . \quad . \quad . \quad (11)$$

where  $V$  denotes a constant dependent on the mechanical properties of the string. If we consider a monochromatic stationary wave of the type :

$$u = ae^{2\pi i(\nu t + \alpha)}, \quad . \quad . \quad . \quad (12)$$

the function  $a$  must satisfy the equation :

$$\frac{d^2 a}{dx^2} + \frac{4\pi^2 \nu^2}{V^2} a = 0, \quad . \quad . \quad . \quad (13)$$

which is of the form (9) with  $\mu = \frac{4\pi^2 \nu^2}{V^2}$  and  $R = 0$ .

The domain  $D$  is here of one dimension formed by the string in its position of equilibrium ; if one end be taken as origin and if  $l$  is the length of the string,  $D$  extends from  $x = 0$  to  $x = l$ , and thus  $a(0) = a(l) = 0$ .

Equation (13) admits of the well-known integral :

$$a = a_0 \sin \left( \frac{2\pi \nu x}{V} + \alpha \right) \quad . \quad . \quad . \quad (14)$$

with two arbitrary constants  $a_0$  and  $\alpha$ . In order to satisfy the boundary conditions we must take  $\alpha = 0$  and  $\frac{2\pi\nu l}{V} = n\pi$ , where  $n$  is an integer, the particular solution becoming :

$$a_n = a_0 \sin \frac{n\pi x}{l}. \quad . \quad . \quad . \quad (15)$$

In this case the proper values are :

$$\mu_n = \frac{n^2\pi^2}{l^2} \quad . \quad . \quad . \quad . \quad (16)$$

and the functions (15) are the corresponding proper functions.

It follows from Fourier's theorem that any state of vibration of the string can be represented by the function :

$$u(x, t) = \sum_n \left( c_n \sin \frac{n\pi}{l} x \cos 2\pi\nu_n t + d_n \sin \frac{n\pi}{l} x \sin 2\pi\nu_n t \right), \quad (17)$$

where  $\nu_n = \frac{nV}{2l}$ , for this function satisfies the wave equation and vanishes at the boundaries. Moreover, by Fourier's theorem it follows that the constants  $c_n$  and  $d_n$  can be chosen so that  $u$  and  $\frac{\partial u}{\partial t}$ , for the value  $t = 0$ , coincide with any two continuous functions vanishing at the boundaries. Since  $u$  satisfies an equation of the second order with respect to the time, this function is determined if  $u$  and  $\frac{\partial u}{\partial t}$  are known for the value  $t = 0$ .

Any state of vibration of the string can thus be represented by (17). Finally, it is a well-known fact that :

$$\int_0^l \sin \frac{n\pi}{l} x \sin \frac{n'\pi}{l} x dx = 0, \quad n \neq n', \quad . \quad . \quad (18)$$

so that the proper functions are orthogonal.

But the proper functions are indefinite to the extent that  $a_0$  is arbitrary in (15). They are said to be normalised when this constant is chosen, so that :

$$\int_D a_n^2 dv = 1. \quad . \quad . \quad . \quad (19)$$

In the case under consideration the normalised functions are :

$$a_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi}{l} x \quad . \quad . \quad . \quad (20)$$

since

$$\int_0^l \sin^2 \frac{n\pi}{l} x dx = \frac{l}{2}.$$

(b) *The Case of a Plane Rectangular Membrane with Fixed Edges.*

The problem to be solved in this case is that of finding a uniform, finite and continuous solution of the equation :

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{1}{V^2} \frac{\partial^2 u}{\partial t^2}, \quad . \quad . \quad . \quad (21)$$

which vanishes at the boundaries of the region D formed by the membrane, i.e. which vanishes for  $x = 0$ ,  $x = A$ ,  $y = 0$ ,  $y = B$ , A and B denoting the sides of the rectangle bounding the membrane.

Let us consider the stationary monochromatic waves of the form :

$$u(x, y, t) = a(x, y) e^{2\pi i(\nu t + \alpha)}. \quad . \quad . \quad (22)$$

We find :

$$\frac{\partial^2 a}{\partial x^2} + \frac{\partial^2 a}{\partial y^2} + \frac{4\pi^2 \nu^2}{V^2} a = 0, \quad . \quad . \quad . \quad (23)$$

which is an equation of the type (9) with  $\mu = \frac{4\pi^2 \nu^2}{V^2}$  and  $R = 0$ .

A solution fulfilling the required conditions is obtained by writing :

$$\mu = \pi^2 \left( \frac{n^2}{A^2} + \frac{n'^2}{B^2} \right), \quad a_{nn'} = \sin \frac{n\pi}{A} x \sin \frac{n'\pi}{B} y. \quad . \quad (24)$$

These are the proper values and proper functions of equation (23). The proper functions are orthogonal, since :

$$\int_0^A \int_0^B a_{nn'} a_{mm'} dx dy = 0 \quad . \quad . \quad (25)$$

except when  $m = n$ ,  $m' = n'$ .

Since  $\int_0^A \int_0^B a_{nn'}^2 dx dy = \frac{AB}{4}$ , the normalised functions are :

$$a_{nn'} = \frac{2}{\sqrt{AB}} \sin \frac{n\pi}{A} x \sin \frac{n'\pi}{B} y. \quad . \quad . \quad (26)$$



It can be shown that the proper values and functions are unique, and that any state of vibration of the membrane can be represented by a function of the form :

$$u = \sum_{nn'} \left( c_{nn'} \sin \frac{n\pi}{A} x \sin \frac{n'\pi}{B} y \cos 2\pi\nu_{nn'} t + d_{nn'} \sin \frac{n\pi}{A} x \sin \frac{n'\pi}{B} y \sin 2\pi\nu_{nn'} t \right), \quad (27)$$

where  $\nu_{nn'} = \frac{V}{2} \sqrt{\frac{n^2}{A^2} + \frac{n'^2}{B^2}}$ , but we shall not give a detailed proof of this.

(c) *The Case of a Plane Circular Membrane with a Fixed Border.*

The centre of the membrane will be taken as origin of a system of polar co-ordinates, and the units chosen so that the radius of the membrane is unity. In this case the wave equation is :

$$\nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} = \frac{1}{V^2} \frac{\partial^2 u}{\partial t^2}, \quad (27)$$

$V$  being a constant characteristic of the membrane.

Let us write :

$$u(r, \theta, t) = a(r, \theta) e^{2\pi i(\nu t + \alpha)}. \quad (28)$$

and thus obtain for  $a$  :

$$\frac{\partial^2 a}{\partial r^2} + \frac{1}{r} \frac{\partial a}{\partial r} + \frac{1}{r^2} \frac{\partial^2 a}{\partial \theta^2} + \frac{4\pi^2 \nu^2}{V^2} a = 0, \quad (29)$$

which is again an equation of the type (9) with  $\mu = \frac{4\pi^2 \nu^2}{V^2}$  and  $R = 0$ . We make the tentative substitution :

$$a = f(r) \phi(\theta). \quad (30)$$

which gives on substitution in (29) :

$$\frac{r^2}{f} \frac{d^2 f}{dr^2} + \frac{r}{f} \frac{df}{dr} + \mu r^2 = - \frac{1}{\phi} \frac{d^2 \phi}{d\theta^2}. \quad (31)$$

The left-hand side of this equation is a function of  $r$  only and the right-hand side of  $\theta$  only, and they can be equal only if they have a constant value  $C$ . Thus :

$$\frac{d^2 \phi}{d\theta^2} = -C\phi, \quad (32)$$

If  $C$  be negative,  $\phi$  is an exponential function of  $\theta$  and  $a$  cannot be uniform in the circular region  $D$ . It follows that  $C$  is positive and the general solution of (32) is :

$$\phi = A \sin (\sqrt{C}\theta + B), \quad . \quad . \quad . \quad (33)$$

$A$  and  $B$  being arbitrary constants. In order that  $\phi$  may be uniform,  $C$  must be equal to the square of some integer  $k$ . We then obtain from (31) :

$$\frac{d^2 f}{dr^2} + \frac{1}{r} \frac{df}{dr} + \left( \mu - \frac{k^2}{r^2} \right) f = 0. \quad . \quad . \quad (34)$$

By changing the variable and substituting  $\rho = \sqrt{\mu} r$  this equation can be written :

$$\frac{d^2 f}{d\rho^2} + \frac{1}{\rho} \frac{df}{d\rho} + \left( 1 - \frac{k^2}{\rho^2} \right) f = 0. \quad . \quad . \quad (35)$$

This is Bessel's equation of order  $k$  and, as is shown in works on analysis, it admits of a single solution which remains finite for  $\rho = 0$  ; this is Bessel's function of order  $k$  which is given by the series :

$$J_k(\rho) = \frac{\rho^k}{2^k k!} \left\{ 1 - \frac{\rho^2}{2(2k+2)} + \frac{\rho^4}{2 \cdot 4(2k+2)(2k+4)} - \dots \right\} \quad (36)$$

We can thus take :

$$f(r) = J_k(\sqrt{\mu} r) \quad . \quad . \quad . \quad (37)$$

but with the condition that  $f(1) = J_k(\sqrt{\mu}) = 0$ . Thus the proper values of  $\mu$  are the squares of the roots of the Bessel function of the  $k$ th order. If  $\alpha_{kn}$  denote the  $n$ th root of  $J_k$ , the proper functions may be written in the form :

$$a_{kn} = J_k(\alpha_{kn} r) \frac{\sin k\theta}{\cos} \quad . \quad . \quad . \quad (38)$$

where  $k$  and  $n$  are integers, the proper values being  $\mu_{kn} = \alpha_{kn}^2$ . The functions (38) are orthogonal, i.e.

$$\int_0^{2\pi} \int_0^1 J_k(\alpha_{kn} r) J_{k'}(\alpha_{k'n} r) \frac{\sin k\theta}{\cos} \frac{\sin k'\theta}{\cos} r dr d\theta = 0 \quad (39)$$

except for  $k = k', n = n'$ .

For  $\int_0^{2\pi} \frac{\sin k\theta}{\cos} \frac{\sin k'\theta}{\cos} d\theta$  is zero if  $k \neq k'$ , and it is still zero when  $k = k'$ , provided that the sine be chosen in one factor

and the cosine in the other ; moreover, it is known from the theory of Bessel functions that :

$$\int_0^1 J_k(\alpha_{kn}r) J_k(\alpha_{kn}r) r dr = 0. \quad . \quad . \quad (40)$$

Thus the integral of the product of two different proper functions is zero.

It can again be shown in this case that the proper values and functions are unique, and that any vibration of the membrane can be represented in the form :

$$u = \sum_{nk} \{ c_{kn} \sin(k\theta + \gamma_{kn}) J_k(\alpha_{kn}r) \sin 2\pi\nu_{kn}t \\ + d_{kn} \sin(k\theta + \delta_{kn}) J_k(\alpha_{kn}r) \cos 2\pi\nu_{kn}t \}, \quad (41)$$

where  $\nu_{kn} = \frac{V}{2\pi} \alpha_{kn}$ .

### 3. A Study of the General Case of Equation (9)

We shall now return to equation (9) in its general form ( $R \neq 0$ ) and seek uniform, finite and continuous solutions vanishing at the boundaries of a certain domain D. Let M be the point with co-ordinates  $(x, y, z)$  ; when it is necessary to call to mind that the value of a function  $f$  is being considered at the point M we shall write  $f(M)$ .

Thus we can write equation (9) in the form :

$$\nabla^2 a(M) + \{\mu - R(M)\}a(M) = 0. \quad . \quad . \quad (42)$$

The determination of the proper values of this equation can be referred to the solution of a homogeneous linear integral equation. This may be shown by beginning with Green's formula :

$$\iiint_D (U \nabla^2 V - V \nabla^2 U) d\tau = \iint_S \left( U \frac{\partial V}{\partial n} - V \frac{\partial U}{\partial n} \right) d\sigma, \quad . \quad (43)$$

where U and V are uniform, finite and continuous functions within the region D bounded by S. The operator  $\frac{\partial}{\partial n}$  is taken along the normal to S, the positive direction being from within the region D outwards.

Let U denote one of the proper functions  $a$  of the equation

in question ; it is by definition uniform, finite and continuous, and is zero on S. For V we shall take :

$$V(M) = G(M, P) = \frac{1}{MP} + v(M, P), \quad . \quad . \quad (44)$$

P being an arbitrarily fixed point within D and  $v(M, P)$  being a uniform, finite function such that  $G(M, P)$  is zero on S and satisfies within D, except at P, the equation :

$$\nabla^2 G(M, P) = R(M)G(M, P). \quad . \quad . \quad (45)$$

In short, we take for V Green's function of the equation  $\nabla^2 f = Rf$  with respect to D at the point P, admitting the existence of this function. In applying (43) we must exclude from the domain D the point P, at which V becomes infinite, by surrounding it by a very small sphere  $\sigma$  and thus  $a(M)$  and  $G(M, P)$  are uniform, finite and continuous in the domain D outside  $\sigma$  ; moreover, they are both zero on S. (43) then gives

$$\iiint_D (a \nabla^2 G - G \nabla^2 a) d\tau = \iint_\sigma \left( a \frac{\partial G}{\partial n} - G \frac{\partial a}{\partial n} \right) d\sigma \quad . \quad (46)$$

Let the radius of  $\sigma$  approach the value zero, the second part of the surface integral tends to zero, since the value of G on  $\sigma$  increases as the inverse of the radius, while the surface decreases as the square of the radius. The first part of the surface integral tends to

$$- a(P) \iint_\sigma \frac{\partial}{\partial r} \left( \frac{1}{r} \right) d\sigma = 4\pi a(P). \quad . \quad . \quad (47)$$

Thus, in the limit :

$$a(P) = \frac{1}{4\pi} \iiint_D (a \nabla^2 G - G \nabla^2 a) d\tau, \quad . \quad . \quad (48)$$

but since according to the definitions the functions  $a$  and G satisfy the relations :

$$\left. \begin{aligned} \nabla^2 a &= (R - \mu)a \\ \nabla^2 G &= RG \end{aligned} \right\} \quad . \quad . \quad . \quad (49)$$

it follows that :

$$a \nabla^2 G - G \nabla^2 a = \mu a G \quad . \quad . \quad . \quad (50)$$

Thus from (48) :

$$a(P) = \frac{\mu}{4\pi} \iiint_D a(M) G(M, P) d\tau, \quad . \quad . \quad (51)$$

this is an integral equation satisfied by the proper function  $a(M)$ . The theory of linear integral equations shows that a homogeneous integral of the type (51) admits of solutions, which are not zero, for certain values of  $\mu_i$  only ; these values, which are infinite in number, are the fundamental constants of the integral equation and the proper values in our vibration problem.

Only a single function,  $a_i$ , determined except for a constant factor, corresponds in general to each of these values,  $\mu_i$  ; the functions  $a_i(M)$  are the fundamental functions of the integral equation and the proper functions in our problem.

When the domain  $D$  is finite, the fundamental constants form a discontinuous series ; on the other hand, when  $D$  extends to infinity, as is the case in quantum problems, there may be a continuous series of fundamental constants. It is sometimes stated that the assembly of fundamental constants forms the spectrum of the integral equation (51) or of the corresponding differential equation (9) because in physics the determination of the fundamental constants corresponds in general with the determination of characteristic vibrations. If the domain  $D$  is of finite extent the spectrum is always a discontinuous spectrum, or a line spectrum ; if it is infinite there may be side by side a line and a continuous spectrum. It remains to show that the proper functions  $a_i(M)$  form in general a system of orthogonal functions. Let  $\mu_i$  and  $\mu_j$  denote two proper values and  $a_i$  and  $a_j$  the corresponding proper functions. Then :

$$\nabla^2 a_i + (\mu_i - R) a_i = 0, \quad \nabla^2 a_j + (\mu_j - R) a_j = 0, \quad (52)$$

whence

$$a_j \nabla^2 a_i - a_i \nabla^2 a_j = (\mu_j - \mu_i) a_i a_j \quad . \quad . \quad (53)$$

and integrating throughout  $D$

$$\int_D (a_j \nabla^2 a_i - a_i \nabla^2 a_j) d\tau = (\mu_j - \mu_i) \int_D a_i a_j d\tau. \quad . \quad (54)$$

By Green's theorem (43) the volume integral is equal to a surface integral over the boundary of  $D$ , and this integral is zero, since the  $a_i$  are by definition zero on this surface.

(54) then gives :

$$(\mu_j - \mu_i) \int_D a_i a_j d\tau = 0. \quad . \quad . \quad (55)$$

Thus the integral throughout  $D$  of the product of two different proper functions is zero ; the conclusion is, however, not valid if several proper functions correspond to the same proper value, for if  $a_i$  and  $a_j$  are two such functions,  $\mu_i = \mu_j$  and it is not possible to deduce from (55) that  $\int_D a_i a_j d\tau = 0$ . This case corresponds exactly to the case of degeneration in the old mechanics where several different motions correspond to the same quantised energy value.

If  $N$  different proper functions ( $a_{i1}, a_{i2}, \dots a_{iN}$ ) correspond to the same proper value, they can always be replaced by  $N$  others, by means of the linear substitution :

$$a'_{ik} = \sum_j c_j^k a_{ij}, \quad (k = 1, 2, \dots N). \quad . \quad . \quad (56)$$

If the  $a'_{ik}$  are to be orthogonal, we require :

$$\int_D a'_{ik} a'_{il} d\tau = \sum_{jm} c_j^k c_m^l \int_D a_{ij} a_{im} d\tau = 0, \quad (l = 1, 2, \dots N). \quad (57)$$

This gives  $\frac{N(N-1)}{2}$  relations for the determination of the  $N^2$  coefficients  $c_j^k$ . It is thus possible to choose  $N$  mutually orthogonal functions for the  $N$  proper functions corresponding to the proper value  $\mu_i$ . In this way the assembly of all the proper functions form an orthogonal system.

The integrals  $\int_D a_i^2 d\tau$  have, of course, always a positive value, and the system of orthogonal functions is said to be normalised when the arbitrary constant factor in each is so chosen that these integrals are equal to unity.

Finally, it can be shown that the normalised proper functions of a partial differential equation with respect to a domain  $D$  possess the property that any function  $f(q_i)$ , uniform, finite and continuous in  $D$  and vanishing at the boundary of this region, can be represented by a series of the form :

$$f(q_i) = \sum_k c_k a_k(q_i). \quad . \quad . \quad (58)$$

If this be admitted the coefficient  $c_k$  can be calculated by multiplying this series by  $a_k$  and integrating throughout D. On account of the orthogonal property of the  $a_i$  we obtain :

$$c_k = \int_D f(q_i) a_k(q_i) d\tau. \quad . \quad . \quad (59)$$

Let us consider the case of quantised systems for which D is an infinite domain, and let A denote an operator. If the function  $Aa_i$  is uniform, finite and continuous and vanishes at infinity, it can be developed as a series of fundamental functions of the form :

$$Aa_i = \sum_k A_{ki} a_k, \quad . \quad . \quad (60)$$

where

$$A_{ki} = \int_D a_k Aa_i d\tau. \quad . \quad . \quad (61)$$

The constants  $A_{ik}$  can be regarded as the terms of a table formed of an infinite number of lines and columns ; they form, in fact, an infinite matrix. We say that  $A_{ik}$  is the element  $ik$  of the matrix corresponding to the operator A.

In the foregoing discussion it has been supposed that the three-space variables entered into the partial differential equation and that D was a domain of three dimensions. The same formulæ are valid if the equation depends upon two variables or only upon one ; the domain D will then be of two dimensions or of one, as in the examples of the preceding paragraph, and the triple integrals may be replaced by double or simple integrals. In the case of the vibrating string, the theorem expressed by formula (58) is Fourier's theorem and (59) reduces to the well-known formula for the coefficients in Fourier's series.

#### 4. The Quantisation of Systems of Particles

Hitherto we have supposed that the system to be quantised is a single particle placed in a given constant field of force ; this is the case with the oscillator and with the hydrogen atom when the reaction of the electron upon the nucleus is neglected. But it may be necessary to apply the process to a system of several particles with mutual interactions ; this, for example, is the case with atoms more complex than that of hydrogen

where a number of electrons are present. The wave equation is then :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial \psi}{\partial q_k} \right) - \frac{8\pi^2}{h^2} F \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t}. \quad (62)$$

If we suppose  $\psi$  to have the form of the stationary wave :

$$\psi = a e^{\frac{2\pi i}{h}(Et + \alpha)}, \quad (63)$$

where  $a$  is a function of the co-ordinates  $q_i$ , the equation in  $a$  is :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a}{\partial q_k} \right) + \frac{8\pi^2}{h^2} (E - F) a = 0. \quad (64)$$

The function  $a$  must be uniform, finite and continuous, and must vanish at infinity in the generalised space where

$$ds^2 = \sum_{ik} \mu_{ik} dq_i dq_k.$$

We shall assume that an infinity of proper values exists for  $E$ , the total energy of the system ; these proper values being the energies in the stable states. To these values proper functions  $a_i$  correspond, and in general there is only one such function to each proper value. When several functions exist for one and the same value, degeneration is said to occur.

It is easy to show that the proper functions are in general orthogonal. For two fundamental values  $E_l$  and  $E_m$  we have :

$$\left. \begin{aligned} \frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a_l}{\partial q_k} \right) + \frac{8\pi^2}{h^2} (E_l - F) a_l &= 0, \\ \frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a_m}{\partial q_k} \right) + \frac{8\pi^2}{h^2} (E_m - F) a_m &= 0, \end{aligned} \right\} \quad (65)$$

whence

$$\begin{aligned} \int_{-\infty}^{\infty} \left\{ \frac{a_m}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a_l}{\partial q_k} \right) - \frac{a_l}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a_m}{\partial q_k} \right) \right\} \sqrt{\mu} dq \\ = \int_{-\infty}^{\infty} \frac{8\pi^2}{h^2} (E_m - E_l) a_l a_m \sqrt{\mu} dq. \quad (66) \end{aligned}$$



where  $dq = dq_1, dq_2 \dots dq_n$  and the integral is  $n$ -dimensional, taken over the whole of the  $q$ -space.

Integrating by parts, the left-hand side becomes :

$$\int \sqrt{\mu} \sum_{ik} \mu^{ik} \left( \frac{\partial a_m}{\partial q_k} \frac{\partial a_l}{\partial q_i} - \frac{\partial a_l}{\partial q_k} \frac{\partial a_m}{\partial q_i} \right) dq,$$

which vanishes, since  $\mu^{ik} = \mu^{ki}$ .

Thus :

$$(E_m - E_l) \int_{-\infty}^{\infty} a_l a_m d\tau = 0. \quad . \quad . \quad (67)$$

When there is a single proper function for each proper value, all the proper functions are orthogonal. If there are several proper functions for each proper value, it will be possible to replace them by the same number of linear combinations and to arrange that the new functions are orthogonal. Moreover, the functions can be normalised by writing  $\int a_k^2 d\tau = 1$ . The system of proper functions can thus always be considered orthogonal and normalised.

Any function  $f(q_1, q_2, \dots, q_n)$  which is uniform, finite and continuous and vanishes at infinity in generalised space can be developed as a series of fundamental functions in the form :

$$f = \sum_k c_k a_k, \quad . \quad . \quad . \quad (68)$$

where

$$c_k = \int_{-\infty}^{\infty} f a_k d\tau. \quad . \quad . \quad (69)$$

Finally, if  $A$  denote a certain operator, and if  $Aa_i$  is uniform, finite and continuous and vanishes at infinity in the space we can write :

$$Aa_i = \sum_k A_{ki} a_k, \quad . \quad . \quad (70)$$

where

$$A_{ki} = \int_{-\infty}^{\infty} a_k Aa_i d\tau.$$

The  $A_{ki}$  are elements of the matrix corresponding to the operator  $A$ .

## CHAPTER XVIII

### SOME EXAMPLES OF QUANTISATION

#### 1. The Plane Rotator

**T**HE simplest case of quantisation is the plane rotator. This is the description of the system formed by a particle of mass  $m$  occupying a circle of radius  $R$ , its position being located by means of a single variable, the azimuth  $\theta$ , the centre of the circle being the origin. Thus, with the ordinary mechanical conceptions :

$$T = \frac{1}{2}mR^2\dot{\theta}^2, \quad p_{\theta} = \frac{\partial T}{\partial \dot{\theta}} = mR^2\dot{\theta} \quad . \quad . \quad (1)$$

and the old method of quantisation gives :

$$\int_0^{2\pi} mR^2 \dot{\theta} d\theta = \int_0^{2\pi} mvR d\theta = nh \quad . \quad . \quad (2)$$

or

$$mvR = \frac{nh}{2\pi}, \quad (n = \text{an integer}), \quad . \quad . \quad (3)$$

whence

$$E_n = T = \frac{1}{2}mv^2 = \frac{n^2\hbar^2}{8\pi^2mR^2} = \frac{n^2\hbar^2}{8\pi^2I}, \quad . \quad . \quad (4)$$

I denoting the moment of inertia of the rotator about the centre. In the new mechanics we must begin with the wave equation :

$$\nabla^2 a + \frac{8\pi^2m}{\hbar^2}(E - F)a = 0, \quad . \quad . \quad (5)$$

which in the present case takes the simple form :

$$\frac{1}{R^2} \frac{d^2 a}{d\theta^2} + \frac{8\pi^2m}{\hbar^2} E a = 0. \quad . \quad . \quad (6)$$

Thus :

$$a = A \sin \frac{2\pi}{h} \sqrt{2mE} R(\theta - \theta_0), \quad (7)$$

$A$  and  $\theta_0$  being the two constants of integration.

In order that this may be a uniform function of  $\theta$ , it is necessary that :

$$2\pi \frac{\sqrt{2mE}}{h} R = n, \text{ or } E_n = \frac{n^2 h^2}{8\pi^2 m R^2} = \frac{n^2 h^2}{8\pi^2 I}. \quad (8)$$

We thus obtain formula (4) again.

The proper functions corresponding to these values are by (7) :

$$a_n = A \sin n(\theta - \theta_0) \quad (9)$$

and the reduced stable waves are :

$$\psi_n = A \sin n(\theta - \theta_0) e^{\frac{2\pi i}{h} (E_n t + \alpha)}. \quad (10)$$

The functions (9) form an orthogonal system, since :

$$\int_0^{2\pi} a_n a_{n'} R d\theta = 0 \text{ if } n \neq n'.$$

If the functions are to be normalised it is necessary to take

$$A = \frac{1}{\sqrt{\pi R}}, \text{ since}$$

$$R \int_0^{2\pi} \sin^2 n(\theta - \theta_0) d\theta = \pi R.$$

The probability cloud in this case corresponding to the stationary wave  $\psi_n$  is at rest, since the velocity,  $\mathbf{v} = -\frac{1}{m} \text{grad } \phi$ , of its elements is zero and the density of the cloud giving the probability of occurrence of the particle is  $A^2 \sin^2 n(\theta - \theta_0)$ .

Instead of considering the stationary wave  $\psi_n$ , we can consider the stable waves :

$$\psi'_n = A' e^{\frac{2\pi i}{h} \{E_n t - \frac{nh}{2\pi} (\theta - \theta_0) + \alpha\}}, \quad (11)$$

obtained by superposing two waves  $\psi_n$ . The probability elements associated with  $\psi'_n$  have the velocity :

$$v = -\frac{1}{mR} \frac{\partial \phi}{\partial \theta} = \pm \frac{1}{mR} \frac{nh}{2\pi}.$$

i.e. by (3) the same velocity as the particle in classical mechanics. The probability of occurrence is in this case the same at all points of the circle.

## 2. The Rotator with a Free Axis

A rather more complicated case is that of the rotator about a movable axis. This consists of a particle of mass  $m$  which rotates on a sphere of radius  $R$  and according to ordinary mechanics it must describe a geodesic or great circle on the sphere. The quantum condition and the formula giving the energy in the stable states in the old quantum theory is thus the same as for the plane rotator.

In wave mechanics we begin with the wave equation :

$$\nabla^2 a + \frac{8\pi^2 m}{h^2} E a = 0. \quad (12)$$

$a$  must be expressed by two variables, the colatitude  $\theta$  and the longitude  $\alpha$ .

On the sphere :

$$ds^2 = R^2 d\theta^2 + R^2 \sin^2 \theta d\alpha^2, \quad (13)$$

the values of the  $g$ 's in this case being :

$$\left. \begin{aligned} g_{11} &= R^2, & g_{12} &= 0, & g_{22} &= R^2 \sin^2 \theta \\ g^{11} &= \frac{1}{R^2}, & g^{12} &= 0, & g^{22} &= \frac{1}{R^2 \sin^2 \theta} \\ g &= R^4 \sin^2 \theta. \end{aligned} \right\} \quad (14)$$

Hence :

$$\nabla^2 a = \frac{1}{\sqrt{g}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{g} g^{ik} \frac{\partial a}{\partial q_k} \right) = \frac{1}{R^2 \sin \theta} \left\{ \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial a}{\partial \theta} \right) + \frac{\partial}{\partial \alpha} \left( \frac{1}{\sin \theta} \frac{\partial a}{\partial \alpha} \right) \right\}, \quad (15)$$

and the final form of the wave equation is :

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial a}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 a}{\partial \alpha^2} + \frac{8\pi^2 m R^2 E}{h^2} a = 0. \quad (16)$$

This equation has been studied and it is known that it has a uniform, finite and continuous solution over the sphere only when the coefficient of  $a$  is equal to the product of two consecutive positive numbers, including zero.

The proper values of  $E$  are therefore :

$$E_n = n(n+1) \frac{h^2}{8\pi^2 m R^2}. \quad (n = 0, 1, \dots) \quad (17)$$

The corresponding proper functions are the spherical functions of Laplace  $Y_n(\theta, \alpha)$ . They can be expressed by means of trigonometrical functions and the Legendre polynomials. The latter are defined by the formula :

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (1-x^2)^n. \quad (18)$$

By means of these we define derived polynomials :

$$P_n^k(x) = (1-x^2)^{\frac{k}{2}} \frac{d^k}{dx^k} P_n(x). \quad (19)$$

The functions of Laplace are given by :

$$Y_n(\theta, \alpha) = \sum_{k=0}^{k=n} (A_k \cos k\alpha + B_k \sin k\alpha) P_n^k(\cos \theta), \quad (20)$$

$A_k$  and  $B_k$  being constants. The stable stationary waves for the rotator can now be written in the form :

$$\psi_{nk}(\theta, \alpha, t) = \sum_{k=0}^{k=n} (A_k \cos k\alpha + B_k \sin k\alpha) P_n^k(\cos \theta) e^{\frac{2\pi i}{h}(E_n t + \gamma)}. \quad (21)$$

It will be noticed in this case that there is degeneration, since for a single value of  $E_n$  it is possible to obtain  $(2n+1)$  different functions by choosing the  $(2n+1)$  constants,  $A_0, A_1, B_1, \dots, B_n$  arbitrarily. The functions  $Y_n$  are orthogonal, since they are the proper functions of a partial differential equation, and therefore the general theorem of the last chapter applies to them.

The probability elements associated with the stationary wave  $\psi_{nk}$  are at rest and their density at a point of the sphere is  $Y_n^2$ . Since several proper functions exist for a single proper value, it is possible to form many linear combinations of stationary waves giving a resultant monochromatic wave. The simplest are of the form :

$$\psi'_{nk} = A' P_n^k(\cos \theta) e^{\frac{2\pi i}{h}(E_n t \pm \frac{k h \alpha}{2\pi} + \gamma)}. \quad (22)$$

The probability elements associated with  $\psi'_{nk}$  describe parallel lines on the sphere with velocity :

$$v = -\frac{1}{m} |\text{grad } \phi| = \frac{k\hbar}{2\pi m R \sin \alpha}.$$

The probability density is a function of the colatitude only, and is equal to  $\{A'P_n^k (\cos \theta)\}^2$ .

More complicated motion could be obtained for the probability elements by combining stationary solutions corresponding to different orientations of the polar axis.

### 3. The Harmonic Oscillator

This case is that of a particle of mass  $m$  constrained to move along a straight line  $Ox$  under a force towards the point  $O$  proportional to the displacement from  $O$  ( $= -kx$ ). In the old mechanics, as we have seen at the beginning of Chapter XVI, the frequency of vibration is independent of the amplitude, and has the value :

$$\omega = \frac{1}{2\pi} \sqrt{\frac{k}{m}} = \frac{1}{T}. \quad . \quad . \quad . \quad (23)$$

The old quantum theory gives for the energy of the stable states :

$$E_n = nh\omega. \quad . \quad . \quad . \quad (24)$$

In the new mechanics the differential equation for the amplitude is :

$$\frac{d^2a}{dx^2} + \frac{8\pi^2m}{\hbar^2} (E - \tfrac{1}{2}kx^2)a = 0. \quad . \quad . \quad (25)$$

Let

$$A = \frac{8\pi^2m}{\hbar^2}, \quad B = \frac{4\pi^2mk}{\hbar^2} = \frac{16\pi^4m^2\omega^2}{\hbar^2}, \quad . \quad (26)$$

so that (25) becomes :

$$\frac{d^2a}{dx^2} + (AE - Bx^2)a = 0. \quad . \quad . \quad (27)$$

Change the variable to  $q$  where :

$$q = B^{\frac{1}{4}}x \quad . \quad . \quad . \quad (28)$$

and let

$$\frac{AE}{\sqrt{B}} = \lambda, \quad . \quad . \quad . \quad . \quad (29)$$

then

$$\frac{d^2a}{dq^2} + (\lambda - q^2)a = 0. \quad . \quad . \quad . \quad (30)$$

The proper values of this equation will be shown to be :

$$\lambda = 1, 3, 5, \dots (2n + 1). \quad . \quad . \quad . \quad (31)$$

After making the substitution :

$$a = e^{-\frac{1}{2}q^2}u \quad . \quad . \quad . \quad . \quad (32)$$

in (30), we obtain :

$$\frac{d^2u}{dq^2} - 2q\frac{du}{dq} + (\lambda - 1)u = 0. \quad . \quad . \quad . \quad (33)$$

Since  $u$  must be uniform, finite and continuous it can be expressed in the form of a series of positive powers of  $q$  :

$$u = c_0 + c_1q + \dots + c_nq^n + \dots \quad . \quad (34)$$

By substitution in (33) and equating to zero the coefficient of  $q^n$  it is found that :

$$c_{n+2} = \frac{2n + 1 - \lambda}{(n + 1)(n + 2)}c_n. \quad . \quad . \quad (35)$$

All the  $c$ 's with an even suffix can be expressed in terms of  $c_0$ , those with an odd suffix in terms of  $c_1$ . The constants  $c_0$  and  $c_1$  are the constants of integration of the equation (33). Let it be supposed in the first instance that  $\lambda$  is an odd number  $(2k + 1)$ , where  $k$  is, of course, even or odd. If  $k$  is even let  $c_1$  be taken equal to zero and let  $c_0$  have any value ; if  $k$  is odd let  $c_0$  be zero and let  $c_1$  have any value. In this way we obtain for  $u$  a polynomial of degree  $k$  known as the  $k$ th polynomial of Hermite and denoted by  $H_k(q)$ . The function  $a = e^{-\frac{1}{2}q^2}H_k$  is uniform, finite and continuous, and has the value zero for  $q = \pm \infty$  ; it is a proper function of equation (30). If  $c_0$  and  $c_1$  be chosen in any other way a finite number of terms will be obtained with an exponent of a particular parity and an infinite number with an exponent of opposite parity, and as  $u$  then tends to infinity more rapidly than  $e^{\frac{q^2}{2}}$  as

$q$  increases indefinitely, the corresponding function  $a$  is not a proper function.

If it be supposed that  $\lambda$  is not equal to an odd integer, whatever the values of  $c_0$  and  $c_1$  a series is obtained for  $u$  which becomes infinite more rapidly than  $e^{\frac{q^2}{2}}$  as  $q$  increases indefinitely, and the corresponding function  $a$  is unsuitable. In short, the differential equation has only a uniform, finite and continuous solution which vanishes at infinity when  $\lambda = 2k + 1$ ,  $k$  being zero or a positive integer. The corresponding proper functions are :

$$a_k(q) = e^{-\frac{q^2}{2}} H_k(q). \quad . \quad . \quad . \quad (36)$$

It is known from the theory of these polynomials that the functions  $a_k$  are orthogonal, but this follows from the general theorem on the orthogonality of proper functions of equations of the type (30). It can also be shown that :

$$\int_{-\infty}^{\infty} H_n^2 e^{-q^2} dq = 2^n n! \sqrt{\pi}, \quad . \quad . \quad . \quad (37)$$

so that when the functions are normalised :

$$a_k(q) = \frac{1}{\pi^{\frac{1}{2}} \sqrt{2^k k!}} e^{-\frac{q^2}{2}} H_k(q). \quad . \quad . \quad (38)$$

Returning to the problem of quantisation, it follows from these results that the proper values of (27) are given by :

$$E_k = (2k + 1) \frac{\sqrt{B}}{A} = (2k + 1) \frac{\hbar \omega}{2} = \left(k + \frac{1}{2}\right) \hbar \omega. \quad (39)$$

This result is remarkable, for we obtain in this way the half quantum expression which was suggested by experiment but which could not be deduced from the old quantum theory. The normalised proper function of (27) corresponding to  $E_k$  is :

$$a_k(x) = \frac{1}{\pi^{\frac{1}{2}} \sqrt{2^k k!}} e^{-\frac{2\pi^2 m \omega}{\hbar} x^2} H_k\left(2\pi \sqrt{\frac{m \omega}{\hbar}} x\right), \quad . \quad (40)$$

and the stationary wave of order  $k$  is :

$$\psi_k(x, t) = \frac{1}{\pi^{\frac{1}{2}} \sqrt{2^k k!}} e^{-\frac{2\pi^2 m \omega}{\hbar} x^2} H_k\left(2\pi \sqrt{\frac{m \omega}{\hbar}} x\right) e^{\frac{2\pi i}{\hbar} \left(k + \frac{1}{2}\right) \omega t}. \quad (41)$$



When the state of the oscillator is represented by  $\psi_k$ , the probability elements are at rest and the probability of occurrence at the point  $x$  is :

$$\frac{1}{2k|k|\sqrt{\pi}} e^{-\frac{4\pi^2 m \omega}{h} x^2} H_k^2\left(2\pi\sqrt{\frac{m\omega}{h}} x\right).$$

The particle can occupy any position along  $Ox$ , but the probability that it is far from the origin is very small. In the old mechanics the motion took place along a limited portion of  $Ox$ , the extremities of this limited strip being the points where the particle turned back along its path. There is thus a great difference in this respect between the old and new mechanics. A harmonic oscillator may be considered in two or three dimensions ; in the latter the particle can be displaced in three directions and with a suitable choice of rectangular axes the potential energy may be written in the form :

$$F = \frac{1}{2}(k_1 x^2 + k_2 y^2 + k_3 z^2). \quad . \quad . \quad (42)$$

Write :

$$\psi(x, y, z, t) = a_1(x) a_2(y) a_3(z) e^{\frac{2\pi i}{h}(E_1 + E_2 + E_3)t}. \quad . \quad (43)$$

The wave equation divides into three equations of the form :

$$\frac{d^2 a_1}{dx^2} + \frac{8\pi^2 m}{h^2} \left(E_1 - \frac{k_1 x^2}{2}\right) a_1 = 0. \quad . \quad . \quad (44)$$

From the result obtained for the linear oscillator it follows that the quantised energy values are :

$$E_{n_1 n_2 n_3} = E_1 + E_2 + E_3 = (n_1 + \frac{1}{2})h\omega_1 + (n_2 + \frac{1}{2})h\omega_2 + (n_3 + \frac{1}{2})h\omega_3, \quad (45)$$

where

$$\omega_i = \frac{1}{2\pi} \sqrt{\frac{k_i}{m}}. \quad (i = 1, 2, 3.) \quad . \quad . \quad (46)$$

The amplitude of the stationary  $\psi$ -waves is expressed as a product of Hermite's polynomials.

If two of the constants  $k_i$  are equal, there is partial degeneration ; if all are equal there is complete degeneration and the oscillator is isotropic. In both cases several quantised energy values coincide ; in other words, there are several stable states for a single proper energy value.

#### 4. The Hydrogen Atom

We now consider the very important case of the hydrogen atom formed by a fixed nucleus of charge  $+e$  and of a planetary electron of charge  $-e$ . We will take a system of spherical co-ordinates about the nucleus;  $\alpha$  = the longitude,  $\theta$  = the colatitude,  $r$  = the radius vector. In spherical co-ordinates we have, for the line element :

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\alpha^2, \quad . \quad . \quad (47)$$

whence

$$\left. \begin{aligned} g_{11} &= 1, & g_{22} &= r^2, & g_{33} &= r^2 \sin^2 \theta, & g_{ik} &= 0 \text{ when } i \neq k, \\ g^{11} &= 1, & g^{22} &= \frac{1}{r^2}, & g^{33} &= \frac{1}{r^2 \sin^2 \theta}, & g^{ik} &= 0 \text{ when } i \neq k, \\ g &= r^4 \sin^2 \theta. \end{aligned} \right\} \quad (48)$$

The equation for  $a$  is therefore :

$$\frac{1}{\sqrt{g}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{g} g^{ik} \frac{\partial a}{\partial q_k} \right) + \frac{8\pi^2 m}{h^2} \left( E + \frac{e^2}{r} \right) a = 0, \quad . \quad (49)$$

which becomes in this case :

$$\begin{aligned} \frac{\partial^2 a}{\partial r^2} + \frac{2}{r} \frac{\partial a}{\partial r} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial a}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 a}{\partial \alpha^2} \\ + \frac{8\pi^2 m}{h^2} \left( E + \frac{e^2}{r} \right) a = 0. \end{aligned} \quad (50)$$

Schrödinger has shown that this equation possesses uniform, finite and continuous solutions, vanishing at infinity, for all positive values of  $E$  and for the negative values :

$$E_n = - \frac{2\pi^2 m e^4}{n^2 h^2}, \quad (n = \text{an integer.}) \quad . \quad (51)$$

The positive proper values correspond to the hyperbolic trajectories of the old mechanics, the negative values correspond to the stable states already obtained by Bohr, for the formula (51) is identical with the fundamental formula of Bohr's theory.

It should be noted that we have a continuous series of proper values prolonging a discontinuous series and we have mentioned that this state of affairs can arise when the domain

D of the problem of proper vibrations is infinite, which is the case here.

The problem presents a case of degeneration; several proper functions correspond to each proper value (51), each requiring for its complete determination two integers,  $k$  and  $k_1$ , such that :

$$0 \leq k < n, \quad 0 \leq k_1 \leq k. \quad . \quad . \quad . \quad (52)$$

According to Schrödinger's calculations, the stationary wave corresponding to the three integers  $n, k, k_1$ , is given by :

$$\psi_{nkk_1}(r, \theta, \alpha, t) = (A \cos k_1 \alpha + B \sin k_1 \alpha) P_k^{k_1}(\cos \theta) x^k e^{-x} L_{n+k}^{2k+1}(x) e^{\frac{2\pi i}{h}(E_n t + \gamma)}, \quad (53)$$

$A, B$  and  $\gamma$  being constants, and  $x$  denoting the quantity  $\frac{4\pi^2 m e^2}{n^2 \hbar^2} r$ . The polynomials  $P_k^{k_1}(\cos \theta)$  were defined in § 2 of this chapter, and the function  $L_{n+k}^{2k+1}(x)$  is a polynomial in  $x$  which depends upon the polynomials of Laguerre, which we will not explain further here.

The probability elements associated with  $\psi_{nkk_1}$  are at rest and the density of the probability cloud is proportional to the square of the amplitude. It should be noted that, as in the case of the oscillator, the electron has a certain probability of being at any distance from the nucleus, but the probability diminishes rapidly with the distance. In the old dynamics, on the other hand, the electron with negative energy  $E_n$  could not lie outside the sphere of radius :

$$R_n = - \frac{e^2}{E_n}, \quad . \quad . \quad . \quad (54)$$

because outside this sphere the kinetic energy would have to be negative, and this would be impossible.

A large number of stable monochromatic waves can be obtained by combining stationary waves of the type (53). It suffices to add together several  $\psi_{nkk_1}$  corresponding to the same value of  $n$ , but with different values of  $k$  and  $k_1$  or with different orientations of the polar axis. One of the simplest combinations is :

$$\psi'_{nkk_1} = A' P_k^{k_1}(\cos \theta) x^k e^{-x} L_{n+k}^{2k+1}(x) e^{\frac{2\pi i}{h}(E_n t \pm \frac{k_1 \hbar}{2\pi} \alpha + \gamma)}. \quad (55)$$

The probability elements associated with the stable wave (55) describe circles about the polar axis with a velocity related to  $r$  and  $\theta$  by the formula :

$$v = -\frac{1}{m} |\text{grad } \phi| = -\frac{1}{mr \sin \theta} \frac{\partial \phi}{\partial \alpha} = \pm \frac{k_1 \hbar}{2\pi mr \sin \theta} \quad (56)$$

which is to be compared with  $mvr = \frac{k_1 \hbar}{2\pi}$  applied by the old quantum theory to the particle itself.

## CHAPTER XIX

### THE MEANING OF THE $\psi$ -WAVES OF QUANTISED SYSTEMS

#### 1. Application of General Principles to Quantised Systems

**T**HE general wave equation for a system subject to no perturbations is

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial \psi}{\partial q_k} \right) - \frac{8\pi^2}{h^2} V \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} \quad . \quad (1)$$

and if the system consists of a single particle as in the cases studied in the last chapter, this reduces to :

$$\frac{1}{m} \nabla^2 \psi - \frac{8\pi^2}{h^2} V \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} \quad . \quad . \quad . \quad (2)$$

Both equations are satisfied by all the linear combinations of the stationary  $\psi$ -waves having frequencies equal to the proper values,  $E_k$  divided by  $h$  ; conversely any uniform, finite and continuous function vanishing at infinity can be expanded as a series of fundamental functions. It is therefore always possible to write :

$$\psi(q_i, t) = \sum_k c_k a_k(q_i) e^{\frac{2\pi i}{h}(E_k t + \gamma_k)}, \quad . \quad . \quad . \quad (3)$$

the functions  $a_k$  being orthogonal and supposed normalised.

The  $c_k$ 's will be supposed to be chosen in such a way that  $\sum_k c_k^2 = 1$ , which is always possible, since  $\psi$  contains a disposable constant factor. In order to explain the meaning of the  $\psi$ -wave we must make use of the two fundamental principles : the principle of interference and of spectral distribution.

According to the former the probability of occurrence of the

particle in space or of the representative point in generalised space is :

$$\begin{aligned}\psi\psi^* &= \sum_{kl} c_k c_l a_k a_l e^{\frac{2\pi i}{h}\{(E_k - E_l)t + \gamma_k - \gamma_l\}} \\ &= \sum_{k_i} c_k^2 a_k^2 + 2 \sum_{k < l} c_k c_l a_k a_l \cos \frac{2\pi}{h}\{(E_k - E_l)t + \gamma_k - \gamma_l\}. \quad (4)\end{aligned}$$

It is rather remarkable that this expression contains exactly the frequencies  $\frac{E_k - E_l}{h}$  which occur in Bohr's theory, and which give the frequencies of the lines of an atomic spectrum as differences of the spectral terms  $\frac{E_k}{h}$ .

The expression (4) gives the absolute probability for on integration :

$$\int \psi\psi^* d\tau = 1, \quad . \quad . \quad . \quad . \quad (5)$$

on account of the relations :

$$\int a_k a_l d\tau = 0, \quad \int a_k^2 d\tau = 1, \quad \sum_k c_k^2 = 1. \quad . \quad . \quad (6)$$

How must we state the principle of spectral distribution in this case ? Born's view is that  $c_k^2$  is the probability that the quantised system, of which the associated wave has the form (3), is to be found after an observation in the stationary state of index  $k$ . In fact, the intensity  $c_k^2 a_k^2$  of the spectral component of frequency  $\frac{E_k}{h}$  in the series (3) is variable from point

to point but the total intensity of this component  $\int c_k^2 a_k^2 d\tau$  is equal to  $c_k^2$ , since the  $a_k$  are normalised and it is therefore natural to regard the  $c_k^2$  as the relative probabilities of the various states of the system associated with the wave (3).

This statement of the principle of spectral distribution for quantised systems appears at first sight to raise a difficulty which it is interesting to examine. We can consider it in its application to a single particle which we will suppose is in any one of its stable states. The probability that it is in the state  $E_k$  is  $c_k^2$ , but when it is in this state the probability that it will

be found at the point  $(x, y, z)$  is  $a_k^2$ , thus by the theorems of total and combined probabilities the probability that the particle is at  $(x, y, z)$  is equal to  $\sum_k c_k^2 a_k^2$ . But this is not equal to  $\psi\psi^*$ , for in (4) the frequency terms occur in addition to this term. It follows that there is a contradiction between the two fundamental principles.

This is the nature of the objection, and to remove it the exact meaning attributed to the  $\psi$ -wave by the theory of Bohr and Heisenberg must be remembered. Our information regarding a quantised system may be summed up in the form of the  $\psi$ -wave of formula (3), but that does not mean that the system is actually in one of the quantised states. The probability the energy state  $E_k$  exists is  $c_k^2$ . A knowledge of the  $\psi$ -wave only tells us that if we make an experiment allowing us to assign a position to the particle in the quantised system the possibility that it lies in the element  $dx dy dz$  is  $\psi\psi^* dx dy dz$ , and if, on the other hand, we make an experiment permitting us to assign an energy state to the particle, there is a probability  $c_k^2$  of finding it in the state  $E_k$ . But it is the essence of the view of Bohr and Heisenberg to admit that these two experiments will affect the initial state of affairs and will affect it in different ways. This is why the application of the theorem of compound probability is not justified. If to determine the position of the particle we begin by finding its energy state and then its position, the probability of finding the particle at  $(x, y, z)$  will be  $\sum_k c_k^2 a_k^2$ ; but there is no reason why this should be the probability of finding the particle at  $(x, y, z)$  by a direct measurement of the position from its initial state since the preliminary determination of the energy disturbs the situation. In short, the interest of this objection is that it shows that if we wish to maintain side by side the two principles of interference and of spectral distribution it is necessary to admit that a quantised system is disturbed by all processes of measurement and of observation.

## 2. The Influence of Perturbations on a Quantised System

We shall suppose that the system is subject to an external perturbation which may depend on the time. The potential

energy  $F(q_i, t)$  consists now of two terms, a term  $V(q_i)$  arising from reactions in the component parts of the system and a term  $R(q_i, t)$  from the external perturbing field.

When this perturbation is absent Schrödinger's equation is :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a}{\partial q_i} \right) + \frac{8\pi^2}{h^2} (E - V) a = 0. \quad (7)$$

The most general  $\psi$ -wave for the system is :

$$\psi = \sum_k c_k a_k e^{\frac{2\pi i}{h} (E_k t + \gamma_k)}, \quad (8)$$

where the  $a$ 's are supposed normalised and  $c_k$  and  $\gamma_k$  are real constants.

When the perturbation is present the equation is :

$$\frac{1}{\sqrt{\mu}} \sum_{ik} \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial \psi}{\partial q_k} \right) - \frac{8\pi^2}{h^2} (V + R) \psi = \frac{4\pi i}{h} \frac{\partial \psi}{\partial t}. \quad (9)$$

The simplest method of obtaining solutions of this equation is to substitute :

$$\psi = \sum_k c_k a_k e^{\frac{2\pi i}{h} (E_k t + \gamma_k)}, \quad (10)$$

and suppose that  $c_k$  and  $\gamma_k$  depend on the time ; this is Dirac's method of variation of the constants. Substituting (10) in (9) we obtain :

$$\begin{aligned} \frac{4\pi i}{h} \sum_k a_k e^{\frac{2\pi i}{h} (E_k t + \gamma_k)} \left( \dot{c}_k + \frac{2\pi i}{h} c_k \dot{\gamma}_k \right) \\ + \frac{8\pi^2}{h^2} R \sum_k c_k a_k e^{\frac{2\pi i}{h} (E_k t + \gamma_k)} = 0. \end{aligned} \quad (11)$$

If we multiply by  $a_l d\tau$  and integrate over the generalised space we obtain :

$$\begin{aligned} \frac{4\pi i}{h} \left( \dot{c}_l + \frac{2\pi i}{h} c_l \dot{\gamma}_l \right) e^{\frac{2\pi i}{h} (E_l t + \gamma_l)} + \frac{8\pi^2}{h^2} \sum_k c_k e^{\frac{2\pi i}{h} (E_k t + \gamma_k)} \\ \int R a_k a_l d\tau = 0. \end{aligned} \quad (12)$$

The integral is the element  $(kl)$  of the matrix which corresponds to the operation of multiplication by  $R$ , and we denote it by



$R_{kl}(t)$ . Thus :

$$\dot{c}_l + \frac{2\pi i}{h} c_l \dot{\gamma}_l = \frac{2\pi i}{h} \sum_k R_{kl} c_k e^{\frac{2\pi i}{h} \{ (E_k - E_l)t + \gamma_k - \gamma_l \}} \quad (13)$$

and the conjugate complex expression is :

$$\dot{c}_l - \frac{2\pi i}{h} c_l \dot{\gamma}_l = - \frac{2\pi i}{h} \sum_k R_{kl} c_k e^{-\frac{2\pi i}{h} \{ (E_k - E_l)t + \gamma_k - \gamma_l \}}. \quad (14)$$

By addition and subtraction of (13) and (14) we obtain the real equations :

$$\dot{c}_l = - \frac{2\pi}{h} \sum_k R_{kl} c_k \sin \frac{2\pi}{h} \{ (E_k - E_l)t + \gamma_k - \gamma_l \} \quad (15)$$

$$c_l \dot{\gamma}_l = \sum_k R_{kl} c_k \cos \frac{2\pi}{h} \{ (E_k - E_l)t + \gamma_k - \gamma_l \}. \quad (16)$$

From these simultaneous equations  $c_l$  and  $\gamma_l$  can be determined if their initial values are known.

According to Born the quantity  $c_k^2$  gives the probability that the system is in the energy state  $E_k$  at time  $t$ .  $\sum_k c_k^2$  is supposed equal to unity at the beginning of the perturbation and must remain equal to unity throughout. It is easy to verify this, for by (15) :

$$\begin{aligned} \sum_l c_l \dot{c}_l &= \sum_l \frac{1}{2} \frac{d}{dt} (c_l^2) \\ &= - \frac{2\pi}{h} \sum_{kl} R_{kl} c_k c_l \sin \frac{2\pi}{h} \{ (E_k - E_l)t + \gamma_k - \gamma_l \}. \end{aligned} \quad (17)$$

and the right-hand side is zero, since a change of sign occurs in any term when the indices  $k, l$  are interchanged ; thus  $\sum_l c_l^2$  is constant and maintains its initial value unity.

Born's hypothesis in the form we have stated it raises a little difficulty. The functions  $\psi_k = a_k e^{\frac{2\pi i}{h} (E_k t + \gamma_k)}$  represent the stationary waves corresponding to the value of the potential energy when the perturbation is non-existent, but at an instant  $\tau$  during the perturbation the potential energy is  $V(q_i) + R(q_i, \tau)$

the proper values and functions at this instant are those of equation :

$$\sum_i \frac{\partial}{\partial q_i} \left( \sqrt{\mu} \mu^{ik} \frac{\partial a}{\partial q_k} \right) + \frac{8\pi^2}{h^2} \{E - V(q_i) - R(q_i, \tau)\} a = 0, \quad (18)$$

where  $\tau$  is regarded as a constant parameter. The proper values  $E_k^\tau$  of this equation must be considered as the energies of stable states at the time  $\tau$ . If an experiment is made at time  $\tau$  to determine the energy of the system, one of the values  $E_k^\tau$  may be found, but there can be no reason why one value  $E_k$  corresponding to the absence of the perturbation should be found. Let  $a_k^\tau$  denote one of the proper functions corresponding to  $E_k^\tau$  for equation (18), then  $\psi$  must be expanded in a series of proper functions in the form :

$$\psi = \sum_k d_k a_k^\tau e^{\frac{2\pi i}{h}(E_k^\tau t + s_k)} \quad . \quad . \quad . \quad (19)$$

The quantity  $d_k^2$  will determine the probability that the system is in the energy state  $E_k^\tau$  at time  $\tau$  (Fock).

If the perturbation has a limited duration beginning at 0 and ending at  $T$ ,  $R(q_i, 0) = R(q_i, T) = 0$ , and consequently  $E_k^0 = E_k^T$ . The coefficients  $c_k$  of (8) may therefore be used to determine the probability that at the end of the perturbation the system is in the state  $E_k$ , the probability being

In this case the difficulty disappears because the proper values of equation (8) have resumed their original values at the end of the perturbation. It will be possible in this way to calculate, as Born does, the probability that the perturbation has brought a system to a particular state. We shall not enter into the developments and applications of these general principles which might well form the subject of a complete volume ; we merely wish to point out how the principle of spectral distribution applies in this case.

### 3. The Probability Cloud and the Heisenberg Matrices

It is impossible to develop here Schrödinger's theory of the emission of radiation by atoms and the method of the Heisenberg matrices. We shall content ourselves with showing how

the matrix elements can be introduced in the simple case of the hydrogen atom by considering the probability cloud associated with the  $\psi$ -wave. In the hydrogen atom there is a single particle and it is sufficient to take three rectangular co-ordinates ( $q_1, q_2, q_3$ ). We shall define the six operations  $Q^i$  and  $P^i$  by the formulæ :

$$\left. \begin{aligned} Q^i &= \text{multiplication by } q_i \\ P^i &= \frac{h}{2\pi i} \frac{\partial}{\partial q_i} \quad (i = 1, 2, 3.) \end{aligned} \right\} \quad . \quad (20)$$

From the definition of the matrix elements corresponding to an operator (Chap. XVII (61)) we obtain the elements with indices  $k, l$  of the six matrices corresponding to  $Q^i$  and  $P^i$  as follows :

$$Q_{kl}^i = \int a_k a_l q_i d\tau, \quad . \quad . \quad . \quad (21)$$

$$P_{kl}^i = \int a_k \frac{h}{2\pi i} \frac{\partial a_l}{\partial q_i} d\tau, \quad . \quad . \quad . \quad (22)$$

the  $a_k$  being normalised proper functions for the hydrogen atom.

Let the wave function for the atom in question be supposed to be :

$$\psi = \sum_k c_k a_k e^{2\pi i(\nu_k t + \gamma_k)}. \quad . \quad . \quad . \quad (23)$$

The density of the corresponding probability cloud is :

$$\rho = a^2 = \sum_k c_k^2 a_k^2 + 2 \sum_{k < l} c_k c_l a_k a_l \cos 2\pi\{(\nu_k - \nu_l)t + \gamma_k - \gamma_l\} \quad (24)$$

and by (37) Chapter IX, the  $q_i$ -component of velocity of the probability elements is :

$$\begin{aligned} v_i &= -\frac{1}{m} \frac{\partial \phi}{\partial q_i} = -\frac{h}{4\pi i m} \frac{\psi^* \frac{\partial \psi}{\partial q_i} - \psi \frac{\partial \psi^*}{\partial q_i}}{a^2} \\ &= \frac{h}{2\pi m a^2} \sum_{k < l} c_k c_l \left( a_k \frac{\partial a_l}{\partial q_i} - a_l \frac{\partial a_k}{\partial q_i} \right) \sin 2\pi\{(\nu_k - \nu_l)t + \gamma_k - \gamma_l\}. \quad (25) \end{aligned}$$

Let the electric charge of the electron be supposed equally divided amongst the probability elements so that the total

charge is :

$$\int \rho e d\tau = e.$$

We may say that the density represents the average probable density of electricity in the atom and the  $q_i$ -component of the electric moment of the probability cloud is :

$$M_i = \int \rho e q_i d\tau = 2 \sum_{k < l} c_k c_l e \int a_k a_l q_i \cos 2\pi\{(\nu_k - \nu_l)t + \gamma_k - \gamma_l\} d\tau. \quad (26)$$

This component contains terms varying periodically with frequencies  $(\nu_k - \nu_l)$ , which are the Bohr frequencies, and the amplitude corresponding to the frequency  $(\nu_k - \nu_l)$  is proportional to  $Q_{kl}^i$ . This indicates a possible physical interpretation of the elements of Heisenberg's matrix  $Q^i$ .

Since the electric density of the cloud varies with the time it is the seat of electric currents. The  $q_i$ -component of the current within the cloud is :

$$J_i = \int \rho e v_i d\tau \quad . \quad . \quad . \quad . \quad (27)$$

and by (25),

$$J_i = \frac{he}{2\pi m} \sum_{k < l} c_k c_l \left( a_k \frac{\partial a_l}{\partial q_i} - a_l \frac{\partial a_k}{\partial q_i} \right) \sin 2\pi\{(\nu_k - \nu_l)t + \gamma_k - \gamma_l\} d\tau$$

= the real part of :

$$\frac{2e}{m} \sum_{k < l} c_k c_l \frac{h}{4\pi i} \int \left( a_k \frac{\partial a_l}{\partial q_i} - a_l \frac{\partial a_k}{\partial q_i} \right) e^{2\pi i\{(\nu_k - \nu_l)t + (\gamma_k - \gamma_l)\}} d\tau. \quad (28)$$

The components of the current are thus decomposed into periodic terms with Bohr frequencies and with amplitudes proportional in a typical case to :

$$\frac{h}{4\pi i} \int \left( a_k \frac{\partial a_l}{\partial q_i} - a_l \frac{\partial a_k}{\partial q_i} \right) d\tau = \frac{h}{2\pi i} \int a_k \frac{\partial a_l}{\partial q_i} d\tau = P_{kl}^i \quad . \quad (29)$$

the equality of the two integral terms following from an integration by parts and the vanishing of the  $a_k$  at infinity. This gives a possible physical interpretation of the Heisenberg matrix components  $P_{kl}^i$ .

It follows also that if  $\delta$  denote the electric density of the probability cloud and  $j_i$  a typical component of the corresponding current :

$$\delta = \rho e = e\psi\psi^* \quad . \quad . \quad . \quad . \quad . \quad (30)$$

$$j_i = \rho e v_i = -\frac{he}{4\pi im} \left( \psi^* \frac{\partial \psi}{\partial q_i} - \psi \frac{\partial \psi^*}{\partial q_i} \right). \quad (31)$$

The formula (30) has been proposed by Schrödinger in his celebrated works on wave mechanics, where he regards  $\delta$  as an actual electric density. (31) was first given by Gordon in a more general form in his memoir on the Compton effect.

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